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Theoretical Computations of Equilibrium Compositions, Thermodynamic Properties, and Performance Characteristics of Propellant Systems

by
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APRIL 1979

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CHINA LAKE, CALIFORNIA 93555

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FOREWORD

This report is an update of a previous report by the same title (NAVWEPS 7043, NOTS TP 2934) published in 1960. Since that time the methodology has been changed; the usage has been changed; new applications have been devised; data banks have been established; and automated usage of data banks has been established. A few minor aspects of the original report have remained unchanged.

This work was performed during fiscal year 1978 under AIRTASK A03W3300/008B/8F31300000 and was checked for technical accuracy by Mr. Stuart Breil.

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(U) *Theoretical Computations of Equilibrium Compositions, Thermodynamic Properties, and Performance Characteristics of Propellant Systems*, by D. R. Cruise. China Lake, Calif., Naval Weapons Center, April 1979, 104 pp. (NWC TP 6037, publication UNCLASSIFIED.)

(U) This report summarizes the methods and equations used in a Naval Weapons Center computer program called the NWC thermochemical program or the propellant evaluation program (PEP). The program is used to calculate high-temperature thermodynamic properties and performance characteristics of propellant systems, and it will handle a maximum of 12 chemical elements and 200 combustion products. Some of the parameters that can be computed with this program are flame temperature, chemical composition, enthalpy, entropy, specific heat ratio and molecular weight of both the combustion chamber and exhaust, frozen and shifting equilibrium, specific impulse, boost velocities, thrust coefficient, characteristic velocity, and exhaust gas velocity. The assumptions made, the limitations imposed, and the input data required for the solution of a specific problem by use of this program are discussed in detail. The appendices provide a working guide for those using the program and give examples of computer inputs.

CONTENTS

INTRODUCTION

The Naval Weapons Center has developed a computer program, often referred to as the NWC thermochemical program or the propellant evaluation program (PEP), for the calculation of high-temperature thermodynamic properties and performance characteristics of propellant systems. This report is a summary of the methods and equations used in the program, which will handle a maximum of 12 chemical elements and 200 combustion products. Flame temperature, chemical composition, enthalpy, entropy, specific heat ratio and molecular weight of both the combustion chamber and exhaust, frozen and shifting equilibrium, specific impulse, boost velocities, thrust coefficient, characteristic velocity, and exhaust gas velocity can be computed with this program. The assumptions made, the limitations imposed, and the input data required for the solution of a specific problem by use of this program are discussed in detail. The appendices provide a working guide for those using the program and give examples of computer inputs.

BACKGROUND

NWC Program Development

The NWC thermochemical program did not come suddenly into being. As early as 1951 thermochemical computations were performed at NWC (formerly NOTS) when Dr. W. S. McEwan and S. Skolnik developed and reported an approach using an analog computer. Dr. D. S. Villars reported his reaction-adjustment method in 1960. The same year H. N. Browne, Jr., completed a program using a method reported by NASA. Mary Williams and Dr. Howard Shomate contributed toward the automation and building of an accurate and usable data bank. In 1964 the author combined some of the ideas of Browne and Villars (who had never collaborated with each other) into the outer skeleton of the Browne program. At the same time a new method of handling condensed species put an end to convergence failures. In 1968 some important suggestions were made by Professors W. R. Smith and R. W. Missen, who had developed their own program at the University of Toronto using the reaction-adjustment method. (A later section of this report is devoted to a discussion of their work.) Since that time the NWC program has continued to evolve in the direction of data automation and new applications.

General Development of Thermochemical Programs

In the past 20 years the computation by high-speed digital computers of high-temperature chemical equilibria has become one of the important applications of computers. It is a challenging application, because of the large sets of nonlinear algebraic equations that must be simultaneously solved and because of the necessity of devising computer codes general enough to handle any particular chemical system[1]. There have been three historic approaches to the problem.

[1]Western States Section of the Combustion Institute. *Proceedings of the First Conference on Kinetics, Equilibria and Performance of High Temperature Systems*, ed. by G. Bahn and E. Zuckowsky. Washington, D.C., Butterworths Scientific Publications, 1960.

One approach, presented by White, *et al.*, is directly motivated by the free-energy criterion for chemical equilibrium[2]. The resulting numerical procedure is the method of steepest descent, which is a general method for the numerical solution of nonlinear algebraic equations.

The second approach, presented by Brinkley[3], uses equilibrium constants and for purposes of background will be described in some detail. First, a "basis" is chosen. A basis is a subset of molecular species (also called components)[4]. It contains as many species as there are chemical elements, and from it all other species may be formed by chemical reaction. A set of equations then establishes the equilibrium relationship of each nonbasis species to the basis. Another set of equations establishes the gram-atom amount of each chemical element. Both sets of equations are solved simultaneously by the Newton-Raphson method, which is a general method for the numerical solution of nonlinear algebraic equations.

Interesting variations in the latter method are presented by Huff *et al.*[5] and Browne[6]. The latter, in particular, introduces the concept of the "optimized" basis, in which the components are present in the greatest possible molar amounts. Browne's computer code for the equilibrium-constant approach was successfully used from 1960 to 1964 by the Naval Weapons Center, then known as the U.S. Naval Ordnance Test Station (NOTS).

The reaction-adjustment method of Villars is the third approach[7,8]. This, too, was a method suggested early in the development of computer codes but not widely used before the development of the present program. Its theory is simple: The chemical system is divided into a number of subsystems, each relating a nonbasis species to the basis. The subsystem with the greatest discrepancy in its equilibrium relationship is corrected stoichiometrically. In this way the gram-atom amounts (chosen correctly at the start) do not change. The reason for convergence is clear: Each iteration is equivalent to arresting all possible reactions but one and allowing that one to proceed according to the law of mass action. This possible (though not plausible) kinetic model can only lead in the direction of equilibrium.

In its computational aspects the method presented by Villars has both advantages and disadvantages. Unlike the former methods, it does not require the inversion of large matrices. This simplifies the coding and reduces the required computer memory. On the other hand, the speed of the method is greatly dependent on the choice of the basis. It is admittedly quite slow when components are chosen that are present only in small molar amounts.

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[2]W. B. White, S. M. Johnson, and G. B. Dantzig. "Chemical Equilibrium in Complex Mixtures." *J. Chem. Phys.*, Vol. 28 (May 1958), pp. 751-5.

[3]S. R. Brinkley, Jr. "Calculation of the Equilibrium Composition of Systems of Many Constituents," *J. Chem. Phys.*, Vol. 15 (1947), pp. 107-10.

[4]H. J. Kandiner and S. R. Brinkley. "Calculation of Complex Equilibrium Relations." *Ind. Eng. Chem.*, Vol. 42 (1950), pp. 850-5.

[5]National Advisory Committee on Aeronautics. *General Method and Thermodynamic Tables for Computation of Equilibrium Composition and Temperature of Chemical Reactions*, by V. N. Huff, S. Gordon, and V. E. Morrell. Washington, D.C., NACA 1951. (NACA Report 1037.)

[6]Naval Ordnance Test Station. *The Theoretical Computation of Equilibrium Compositions, Thermodynamic Properties and Performance Characteristics of Propellant Systems*, by H. N. Browne Jr., M. M. Williams, and D. R. Cruise. China Lake, Calif., NOTS, 1960. (NAVWEPS Report 7043, NOTS TP 2434, publication UNCLASSIFIED.)

[7]D. S. Villars. "A Method of Successive Approximations for Computing Combustion Equilibria on a High Speed Digital Computer," *J. Chem. Phys.*, Vol. 63 (1959), pp. 521-5.

[8]D. S. Villars. "Computation of Complicated Combustion Equilibria on a High-Speed Digital Computer," in *Proceedings of the First Conference on Kinetics, Equilibria and Performance of High Temperature Systems*, ed. by G. Bahn and E. Zuckowsky. Washington, D.C., Butterworths Scientific Publications, 1960.

It was decided to try Villars' method and to choose an optimum basis by Browne's method. The automatic choosing of the optimum basis is not difficult to code, and it serves two purposes: It greatly speeds convergence, and it relieves the user of the burden of choosing the basis himself.

ORGANIZATION OF REPORT

The next three sections of this report describe the combination of Villars' and Browne's methods for computing a chemical composition at a given pressure and temperature. The description is divided into three parts. The first part presents in detail the basis optimization technique used, which differs only slightly from that reported by Browne. The second part presents the procedures for determining equilibrium, which follow essentially the method of Villars, except for some suitable modifications to increase computing speed. The third part presents certain manipulations with condensed phases that increase the generality of the method. The remaining five sections describe various aspects of the method. For a concise presentation, the procedures are described in the notation of linear algebra.

The appendices describe how to run the program on the computer.

BASIS OPTIMIZATION

Consider a system which contains S chemical elements and N molecular species such that N is greater than S. Relating the species to the elements is a molecular composition matrix C. Here the individual elements c_{ik} state how many atoms of the kth element are contained in a molecule of the ith species.

Let any arbitrary choice of S molecular species be denoted

$$i(j) \qquad 1 \leqslant j \leqslant S$$

where the subset of i's chosen is considered to be a function of a dummy index j. A basis is formed by $i(j)$ if and only if the following relationship exists:

$$|B| \neq 0 \tag{1}$$

where the vertical bars denote the determinant of the matrix B and where the elements of B are defined as follows:

$$b_{jk} = c_{i(j),k} \qquad \begin{matrix} 1 \leqslant j \leqslant S \\ 1 \leqslant k \leqslant S \end{matrix} \tag{2}$$

Equation 2 involves three indexes, i, j, and k, where i is not independent because of its functional relationship to j. This equation describes the formation of the square basis matrix B by extracting some of the rows of the larger, composition matrix C, namely those rows corresponding to the chosen species.

The optimization problem requires that $i(j)$ be chosen to form a basis and that the corresponding molar amounts $n_{i(j)}$ be as large as possible. This can be done by a process of trial and error. First the molecular species must be so sorted that the molar amounts are in descending order. Here the species subscript i becomes itself a function of a subscript m, such that

$$n_{i_1} \geq n_{i_2} \geq \cdots \geq n_{i_m} \geq n_{i_{m+1}} \geq \cdots \geq n_{i_N} \tag{3}$$

The basis is now found as follows. First i_1 is chosen to be the first basis species and the i_1st row of the C matrix is put into the first row of the B matrix. Next the j and m indexes are set to the value 2. The third step is to test i_m as an acceptable basis species. This is done by inserting the i_mth row of the C matrix into the jth row of the thus far incomplete B matrix. If there is linear dependence among the rows of the incomplete B matrix, the test fails, and the m index is increased by unity. If there is no linear dependence, i_m becomes the jth basis species, which is to say, $i(j)$ and both the j and m indexes are increased by unity. From here the process returns to the third step until $i(S)$ is determined.

Browne established linear dependence by the following relationship:

$$\left| (B^{inc})\,(B^{inc})^T \right| = 0 \tag{4}$$

where T denotes transposition and B^{inc} is the incomplete B matrix. However, it was found that the test could be performed much faster by using the Gram-Schmidt construction. This construction is expressed as follows:

$$b'_{\ell k} = b_{\ell k} - \left(\sum_{h=1}^{S} b_{\ell h} b_{nh} \Big/ \sum_{k=1}^{S} b^2_{\ell h} \right) b_{nk} \begin{cases} 2 \leq \ell \leq j \\ 1 \leq n \leq j - 1 \\ 1 \leq k \leq S \end{cases} \tag{5}$$

where $b'_{\ell k}$ replaces the element $b_{\ell k}$ and n and ℓ are dummy indexes. If all elements of the jth row are zero after the construction, there is linear dependence, and the test fails. The underlying theory of linear dependence and the Gram-Schmidt construction are presented in Stoll[9] and other texts on linear algebra.

The complete B matrix is determined at the end of the optimization process, and the ν matrix of reaction coefficients is expressed

$$\nu = CB^{-1} \tag{6}$$

Equilibrium constants may then be computed from the elements of the ν matrix as follows:

$$\ln K_i = \frac{-1}{RT} \left[g_i - \sum_{j=1}^{S} \nu_{ij}\, g_{i(j)} \right] \tag{7}$$

where g_i is the standard Gibbs free energy of the ith species at the given temperature T.

[9] R. Stoll. *Linear Algebra and Matrix Theory*. New York, McGraw-Hill, 1952. Chapter 8, especially section 8.7.

PROCEDURES FOR DETERMINING EQUILIBRIUM

The equilibrium procedure requires that a first estimate of the equilibrium composition be given. This estimate need not closely approximate the final solution, but it must express the desired gram-atom amount of each chemical element. This expression can be accomplished in many ways. One way, easy to code, is to set the molar amount of one monatomic species of each chemical element to the desired gram-atom amount, then set the molar amounts of the rest of the species at zero (or at negligibly small values). This particular way requires that the monatomic species appear in the formulation.

The general iterative procedure assumes that the gram-atom amounts are correct and that the optimum basis has been chosen for the current estimate of the molar amounts. The reaction coefficient matrix, ν, and the array of equilibrium constants, K_i, are therefore available from Equations 6 and 7. A pass is made through the reaction (nonbasis) species to determine whether the proper equilibrium relationships are met. If not, the molar amounts, n_i, are stoichiometrically corrected. The basis is again optimized whenever the current basis is no longer optimum. The details are described below using the conventions of Prigogine[10]

The chemical reaction which yields the ith reaction species from the basis may be written as

$$\sum_{j=1}^{S} \nu_{ij} i(j) \rightarrow i \tag{8}$$

therefore, a stoichiometric change in the extent of reaction, $\Delta\xi$, causes the following alterations in composition.

$$n_i' = n_i + \Delta\xi \tag{9}$$

$$n_{i(j)}' = n_{i(j)} - \nu_{ij}\Delta\xi \qquad 1 \leqslant j \leqslant S \tag{10}$$

where the primed n_i denotes the molar amounts after the change. This change, by definition, does not alter the gram-atom amount of any chemical element.

Basis optimization guarantees that n_i is smaller than any of the $n_{i(j)}$ in the basis for which $\nu_{ij} \neq 0$. In actuality most reaction species are smaller in molar amount by many orders of magnitude than the basis species from which they are formed. The gaseous species more than two order of magnitude smaller are arbitrarily classified as *minor* species, and the rest of the nonbasis species, including condensed species of any molar amount, are classified as *major* species.

The correct equilibrium relationship for the ith reaction is expressed as

$$-\sum_{j=1}^{S} \gamma_{i(j)}\, \nu_{ij}\, \ell n\, (An_{i(j)}) + \gamma_i\, \ell n\, (An_i) = \ell n\, K_i \tag{11}$$

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[10] I. Prigogine and R. Defay. *Chemical Thermodynamics*, translated by D. Everett. London Longmans, Green and Co., 1954.

where the phase parameter γ_i takes the value unity if the ith species is a gas and the value zero if it is condensed, and

$$A = \frac{P}{\sum_{i=1}^{N} \gamma_i n_i}$$

where P is the given pressure. If the current molar guesses are incorrect, the terms on the left will equal some value other than $\ln K_j$ and are denoted $\ln Q_j$. The iterative procedure obviously must adjust the values of n_j until the values of Q_j approach those of K_j within a specified tolerance. The log of the equilibrium constant may be differentiated with respect to the reaction parameter ξ (assuming A to be constant), yielding

$$\left(\sum_{j=1}^{S} \gamma_{i(j)} \nu_{ij}^2 / n_{i(j)} + \gamma_i / n_i \right) d\xi = d(\ln K_j) \tag{12}$$

An estimate of the stoichiometric correction for a major species is obtained by applying Newton's method of locating roots, which is expressed by the following approximate form of Equation 12:

$$\Delta\xi \cong (\ln K_j - \ln Q_j) / \left(\sum_{j=1}^{S} \gamma_j \nu_{ij}^2 / n_{i(j)} + \gamma_i / n_i \right) \tag{13}$$

Equations 9 and 10 are then applied. (In practice, $\Delta\xi$ is not allowed to take values leading to negative n_j.) All major species are corrected by this method during the iteration pass. This differs from the method used by Villars, who applied the correction only where the discrepancy $|\ln K_j - \ln Q_j|$ was greatest. The modification is justified for two reasons—(1) little additional computing time is required to actually make the correction after the discrepancy is determined, and (2) the basis optimization has minimized the interaction effect that a given correction has on the other equilibrium relationships.

An estimate of the stoichiometric correction for minor species is obtained as follows:

$$n_i' \cong n_i \, (K_i / Q_i) \tag{14}$$

$$\Delta\xi = n_i' - n_i \tag{15}$$

Equation 10 is then applied. This approach assumes that the error in K_i is contained entirely in the value of n_i. This is nearly true for minor species, because a large relative change in n_i is accomplished by a small $\Delta\xi$, and there is no appreciable change in the basis. This separate analysis of minor species also differs from that of Villars. Again there are advantages. Equations 14 and 15 require less computing time than Equation 13. Then, too, the former equations compute the molar amounts of the minor species to a high degree of accuracy (four or more significant decimal places) even when the relative molar amounts are quite small (e.g., 10^{-10} or 10^{-20}). (This is useful in some applications involving ionic species.) It was also found that computer time is saved by correcting the minor species only on every fourth iteration pass, unless convergence is attained among the major species in the meantime. The variable A, defined above, is computed once at the start of every iteration pass.

Convergence was considered to be attained when all *binding* equilibrium relationships passed the following tests:

$$\text{(major species)} \quad \left| (1 - K_i/Q_i) \right| \leq 10^{-5} \tag{16}$$

$$\text{(minor species)} \quad \left| (1 - K_i/Q_i) \right| \leq 10^{-4} \tag{17}$$

However, not all equilibrium relationships are binding. This is discussed in the next section.

DELETION OF CONDENSED PHASES

The formulation of the chemical equilibrium problem, as usually presented, is not general enough to completely describe the behavior of condensed phases. To overcome this weakness special procedures must be used. The following two procedures are particularly suited to the method of determining equilibrium presented above.

When the computed amount of a condensed species becomes negligibly small (say, 10^{-6}) and $\ell n\ K_i - \ell n\ Q_i$ is negative, no correction is applied, and the equilibrium relationship is no longer binding. In this way a phase is deleted and a degree of freedom is gained in accordance with the phase rule [11].

When a reaction occurs entirely among condensed species, the denominator in Equation 13 is zero. In this situation the phase rule states that at least one of the involved species cannot be present in any molar amount (if we are free to specify pressure and temperature). The situation is handled by ignoring Equation 13 and determining a value of $\Delta\xi$ that takes the sign of $\ell n\ K_i - \ell n\ Q_i$ and that has a magnitude not leading to negative molar amounts when Equations 9 and 10 are applied. This is symbolically expressed as

$$\Delta\xi = \text{sign}\ (\ell n\ K_i - \ell n\ Q_i)\ \min \left[n_i,\ n_{i(1)}/|\nu_{i1}|,\ n_{i(2)}/|\nu_{i2}|, \ldots\ n_{i(S)}/|\nu_{iS}| \right] \tag{18}$$

In this manner the molar amount of at least one condensed species is reduced to zero.

When these procedures were included in the computer code, correct solutions were obtained even in extremely difficult cases. In fact, correct solutions can be obtained where no gas phase is present.

[11] A. Findlay. *Phase Rule*. New York, Dover, 1951.

NUMERICAL EXAMPLES OF BASIS AND EQUILIBRIUM CALCULATIONS

Consider a system containing 1 gram-atom of carbon and 2 gram-atoms of oxygen. The following combustion species may be chosen and associated with the composition matrix shown below:

i	Species	C	O
1	C	1	0
2	C_3	3	0
3	O	0	1
4	O_2	0	2
5	CO	1	1
6	CO_2	1	2
7	C(graphite)	1	0

$= C$ (composition matrix)

One way to choose the initial composition guess is to set the monatomic gases to the desired gram-atom amounts and the rest of the species to zero as follows:

Species	i	n_i
C	1	1.0
C_3	2	.0
O	3	2.0
O_2	4	.0
CO	5	.0
CO_2	6	.0
C(graphite)	7	.0

Obviously the best basis for these composition values is:

Species	i	$i(j)$
C	1	1
O	2	3

for these are the species in greatest concentration from which all other species may be formed. This is the basis the program would use on the first iteration.

For a more interesting example of a basis calculation, let us say that at a later iteration the current composition guesses are:

Species	i	n_i
C	1	0.4874996
C_3	2	0.0045000
O	3	0.5005000
O_2	4	0.5000000
CO	5	0.4985000
CO_2	6	0.0005000
C(graphite)	7	0.0000004

(If previous calculations are correct, these values will still reflect the proper gram-atom amounts of C and O.)

These may be sorted into the order of decreasing molar concentration:

Species	m	i_m	n_{i_m}
O	1	3	0.5005000
O_2	2	4	0.5000000
CO	3	5	0.4985000
C	4	1	0.4874996
C_3	5	2	0.0045000
CO_2	6	6	0.0005000
C(graphite)	7	7	0.0000004

Species i_1 (O) is immediately chosen as the first basis species and the i_1st (here the third) row is taken from the composition matrix to become the first row of the basis matrix.

$$\begin{bmatrix} 0 & 1 \end{bmatrix} = B^{inc}$$

Next the i_2nd (here the 4th) row of the C matrix is placed into the B matrix:

$$\begin{bmatrix} 0 & 1 \\ 0 & 2 \end{bmatrix} = B \text{ (to be tested)}$$

Although linear dependence is obvious in this case, the program actually performs the Gram-Schmidt construction which transforms the second row as follows:

$$b'_{21} = b_{21} - \left(\frac{\Sigma b_{2h}\, b_{1h}}{\Sigma b_{1h}^2} \right) b_{11} = 0 - \frac{0+2}{0+1} \cdot 0 = 0$$

$$b'_{22} = b_{22} - \frac{\Sigma b_{2h}\, b_{1h}}{\Sigma b_{1h}^2} b_{12} = 2 - \frac{0+2}{0+1} \cdot 1 = 0$$

Because both elements of the transformed row are zero, O_2 is rejected as a basis species.

Next i_3 (CO) is tested as the basis species. The i_3rd row (here the 5th) of the composition matrix is placed into the second row of the basis matrix:

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} = B \text{ (to be tested)}$$

Gram-Schmidt construction transforms the first element of the second row as follows:

$$b'_{21} = b_{21} - \frac{\Sigma b_{2h}\, b_{1h}}{\Sigma b_{1h}^2} \qquad b_{11} = 1 - \frac{0+1}{0+1} \cdot 0 = 1$$

This element is non-negative and CO is immediately accepted as a basis species without further calculations. Also, because there are now as many basis species, as there are elements (B is square), the basis is complete and because of the above technique, "optimized."

The results are summarized thus:

Species	j	$i(j)$	m	i_m
O	1	3	1	3
CO	2	5	3	5

The next step is to find the inverse of the B matrix which is

$$B^{-1} = \begin{bmatrix} -1 & 1 \\ 0 & 0 \end{bmatrix}$$

The ν matrix of reaction coefficient is now found as follows:

$$\nu = CB^{-1} = \begin{bmatrix} 1 & 0 \\ 3 & 0 \\ 0 & 1 \\ 0 & 2 \\ 1 & 1 \\ 1 & 2 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} -1 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} -1 & 1 \\ -3 & 3 \\ 1 & 0 \\ 2 & 0 \\ 0 & 1 \\ 1 & 1 \\ -1 & 1 \end{bmatrix}$$

The coefficients may be verified by noting that the following chemical equations balance:

i						
1	(-1)	O	+	(1)	CO	$\longrightarrow$ C
2	(-3)	O	+	(3)	CO	$\longrightarrow$ C_3
3	(1)	O	+	(0)	CO	$\longrightarrow$ O
4	(2)	O	+	(0)	CO	$\longrightarrow$ O_2
5	(0)	O	+	(1)	CO	$\longrightarrow$ CO
6	(1)	O	+	(1)	CO	$\longrightarrow$ CO_2
7	(-1)	O	+	(1)	CO	$\longrightarrow$ C(graphite)

These coefficients may be used to determine the equilibrium constants for each reaction. For instance for the first reaction

$$\ell n\ K_1 = \frac{-1}{RT}\ [g_C - [(-1)\ g_O + (1)]\ g_{CO}]$$

where g is the given Gibbs free energy at the given temperature T.

Let us say for the sake of an example that T = 5500 K and P = 1 atm and that the equilibrium constants computed by the above method turn out to be

Reaction	$\ell n\ Ki\ (5500)$
1	-1.4
2	-5.95
3	0
4	---
5	0
6	---
7	-3.91

The variable A, which converts molar concentrations to partial pressures, is computed as follows:

$$A = P/\sum_{i=1}^{6} \gamma_i n_i \text{ (summation to be taken only over gases)}$$

$$A = 1/(0.4874996 + 0.0045 + 0.5005 + 0.5 + 0.4985 + 0.0005)$$

$$A = 1/1.9914996 = 0.5022 \text{ (rounded)}$$

Since all products involved are gases, $\ell n\ Q$ for the first reaction is computed thus:

$$\ell n\ Q = -\Sigma\ \nu_{ij}\ \ell n\ (An_{i(j)}) + \ell n\ A\nu_i$$

$$= [(-1)\ \ell n\ (0.5022 \cdot n_{CO}) + (+1)\ \ell n\ (0.5022 \cdot n_O)] + \ell n\ (0.5022 \cdot n_C)$$

$$= + \ell n \left[\frac{0.4975\ (0.5005)\ (0.5022)}{0.4985}\right] = -1.3829$$

The molar amount of C is not less than one hundreth of that of CO or O, so the formula for the correction of a major species is used:

$$\Delta\xi = (\ell n\ K_1 + \ell n\ Q_1)\ /\ (\Sigma\ \nu_{ij}^2/n_{i(j)} + 1/n_i)$$

$$\Delta\xi = (-1.4 + 1.3829)/\left(\frac{(-1)^2}{n_O} + \frac{(+1)^2}{n_{CO}} + \frac{1}{n_C}\right)$$

$$\Delta\xi = (-0.0171)/6.055 = -0.0028$$

The corrections in composition are now made as follows:

Species	
O	$n'_O = 0.5005 - (-1)(-0.0028) = 0.4977$
CO	$n'_{CO} = 0.4985 - (+1)(-0.0028) = 0.5013$
C	$n'_C = 0.4975 - 0.0028 = 0.4947$

(These new values may be substituted into the expression for $\ell n\ Q$ above yielding -1.4004, which is a significantly better estimate of $\ell n\ K_1$.)

Next, we turn to the second reaction

$$(-3)\ O + (3)\ CO \longrightarrow C_3$$

Because $nC_3 = 0.0045$ is less than 0.01 of the smallest ($n_O = 0.4977$) concentration of the basis species, C_3 is classified as minor.

The equilibrium constant is given as $\ell n\ K = -5.95$ or $K = 0.002605$ and Q is evaluated by

$$Q_2 = \frac{(0.5022\ n_O)^3\ (0.5022\ n_{C_3})}{(0.5022\ n_{CO})^3}$$

$$= \frac{(0.5022)\ (0.4977)^3\ (0.0045)}{(0.5013)^3} = 0.0002212$$

(Note that the new values of n_O and n_{CO} are used.) The new concentration of C_3 is found by the formula for minor species.

$$= 0.0045 \left(\frac{0.002510}{0.002212} \right) = 0.0053$$

The change in the basis species is then determined

$$\Delta\xi = 0.0053 - 0.0045 = 0.0008$$

$$n'_O = 0.4977 - (-3)\ 0.0008 = 0.5001$$

$$n'_{CO} = 0.5014 - (+3)\ 0.0008 = 0.4990$$

(Again, a reevaluation of Q shows a greatly improved estimate of K.)

The third reaction

$$(1)\ O + (0)\ CO \longrightarrow O$$

simply shows the formation of a basis species from itself and so it is ignored.

Reactions four through six fall into the same categories as the first three and so will not be illustrated here.

The seventh reaction (-1) O + (+1) CO ⟶ C(graphite) shows the formation of a condensed species, and so it is considered to be major even though its concentration is well under 1/100 of the smallest basis species. $\ell n\ Q$ is found as follows:

$$\ell n\ Q_3 = (-1)\ \ell n\ (An_O) + (+1)\ \ell n\ (An_{CO})$$

$$= -\left[(-1)\ \ell n\ (0.5022)\ (0.5001) + (+1)\ \ell n\ (0.5022)\ (0.4990)\right]$$

$$= \ell n\ \frac{0.5001}{0.4990} = 0.0022$$

(No term involving $n_{C(graphite)}$ appears in this expression because C(graphite) is a nongas.)

Normally this species would be corrected as before for a major species. But the following conditions exist:

$$n_{C(graphite)} < 0.000001, \text{ and } \ell n\ K_7 - \ell n\ Q_7 \text{ is negative}$$

Therefore, no correction is made and the equilibrium relation is not binding.

The procedure outlined is repeated for all species until all binding equilibrium relations are satisfied to a specified tolerance.

THE WORK OF SMITH AND MISSEN

Professors Smith and Missen at the University of Toronto reported further results on the reaction-adjustment method in 1968.[12] Their work points out that a convergence forcer is required for the method. It was an oversight that this had not been reported in the work by the author.[13] A device to force convergence is indeed required.

The NWC program computes limits on $\Delta\xi$

$$\Delta\xi_{min} \leq \Delta\xi \leq \Delta\xi_{max} \tag{19}$$

such that negative concentrations do not occur. It forces convergence by narrowing these limits as follows:

$$1/2\Delta\xi_{min} \leq \Delta\xi \leq 1/2\Delta\xi_{max} \tag{20}$$

Empirically this has been found to work.

Smith and Missen use a more elegant technique, which in effect tests the results of each reaction adjustment to ensure that the free energy minimum has not been passed over. If this occurs, they reduce the extent of the adjustment.

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[12] W. R. Smith and R. W. Missen. "Calculating Complex Chemical Equilibria by an Improved Reaction-Adjustment Method," *Can. J. Chem. Eng.*, Vol. 46 (1968), pp. 269-72.

[13] D. R. Cruise. "Notes on the Rapid Computation of Chemical Equilibria," *J. Phys. Chem.*, Vol. 68 (1964), pp. 3797-802.

Smith and Missen also report that faster convergence can be achieved by obtaining a better initial estimate of the composition.

Smith and Missen further draw parallels between the reaction-adjustment method and linear programming. This inspired the author to update the basis by the tableau method of linear programming[14] instead of the more time consuming Gram-Schmidt construction previously reported (footnote 13). This updated version works by testing each species after adjustment to determine if it is now larger than any of the basis species with which it reacts. If so, the two are interchanged, and the equations are updated as suggested by the tableau format (footnote 14).

NOTES ON THE PROPELLANT MODEL

A theorem by Duhem (see Chapter XIII of *Chemical Thermodynamics*[10]) states that "Whatever the number of phases, of components, or of chemical reactions, the equilibrium state of a closed system for which we know the initial masses is completely determined by two independent variables." This determination is made by the NWC thermochemical program in the theoretical evaluation of propellant performance. In the mathematics of the program the independent variables chosen are pressure and temperature. Two other variables of interest and possible choices for independent variables are enthalpy and entropy. These too, however, are computed from equilibrium compositions and are therefore dependent on pressure and temperature in this program. Desired value of entropy or enthalpy are achieved by repeating the above determination for various temperatures, and new temperature guesses are obtained by interpolation.

Theoretical propellant evaluation is based on a straightforward thermodynamic model consisting of two processes: (1) constant pressure, adiabatic *combustion* and (2) isentropic, adiabatic *expansion*.

The assumptions behind the combustion process include

1. Reaction kinetics are fast enough that chemical equilibrium is attained before the products leave the combustion chamber and enter the nozzle.*
2. No heat exchange occurs between the propellant system and the surroundings.**
3. Gaseous species individually obey the perfect gas law and collectively obey Dalton's law of partial pressures.

When such assumptions are made, the system enthalpy and the system pressure completely determine the final state and chemical composition of the system after combustion. The solution to this state and composition is found by a computing technique called "enthalpy balance." The method used by the propellant evaluation program is described below.

The system enthalpy itself is determined by the propellant heat of formation, which (excluding heats of mixing) is a linear weighting of the heats of formation of the individual propellant

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[14] G. Hadley. *Linear Programming*, 2nd ed. Reading, Mass., Addison Wesley, June 1963. Pp. 126 ff.

* Real propellants for which this assumption is not valid are said to "burn on the wrong side of the nozzle." This may be referred to as a Type I inefficiency and is one of the principle reasons for disagreement between the program and reality.

** In ramjets, the stagnation energy of the incoming air becomes part of the system. This may simply be added to the heat of formation of air.

ingredients. The value of enthalpy does not change during combustion, so this is also the value of the system enthalpy after combustion. By definition, system enthalpy is the heat needed to form the system in its current state from the elements in their most natural state at 298K and one atmosphere.

The assumptions behind the expansion process include: (1a) Reaction kinetics fast enough that chemical equilibrium is maintained throughout expansion, i.e., the shifting hypothesis; (1b) reaction kinetics so slow that no appreciable change occurs in the chemical composition during expansion, i.e., the frozen hypothesis; (2) expansion process is reversible*; (3) no heat exchange between system and surroundings; and (4) gaseous species individually obey the perfect gas law and collectively obey Dalton's law and nongases occupy no volume.

When such assumptions are made, the system entropy and the system pressure completely determine the final state of the system, regardless of the path. The solution of this state and composition is found by a computing technique called entropy balance. The latter differs little from enthalpy balance. (System entropy is referenced to the third law of thermodynamics.)

The need for the techniques described below arise because the chemical equilibrium problem is formulated to calculate composition and state from given pressure and temperature values. The calculation of performance and design parameters, however, demand that the propellant model above be utilized.

The first problem is to find the value of temperature at which a given enthalpy and pressure requirement is satisfied. This provides the "adiabatic flame temperature" and, as a by-product, the system entropy. The second problem is to find the value of temperature which satisfies the system entropy at a given exhaust pressure. In both cases, pressure is entered directly into the equilibrium code and temperature guesses must be introduced until the enthalpy or entropy conditions are satisfied.

Enthalpy and entropy are each monotonic functions of temperature; their functional values always increase with increasing temperature. In ideal cases, they are smooth, nearly linear curves. In less frequent, but certain to occur, cases the curves are actually discontinuous. This occurs at the fusion temperatures of condensed species.

Two numerical methods suggest themselves: Newton's method and the interval-halving method.

Newton's method consists of correcting successive temperature guesses by the following formula:

$$T_i = T_{i-1} - f(T_{i-1})/f'(T_{i-1}) \tag{21}$$

where T_i is the new guess, T_{i-1} is the previous guess, $f(T)$ is $H(T) - H_0$ in the case of enthalpy balance, and $f(T)$ is $S(T) - S_0$ in the case of entropy balance. H_0 and S_0 are the desired values of enthalpy and entropy. The derivative in the case of enthalpy is expressed as $f'(T) = C_p$ and in the case of entropy $f'(T) = C_p/T$.

Newton's method is very rapid when the curve is fairly straight and when a good guess is given. There is no guarantee of its convergence. It definitely will not converge in areas where the curve is discontinuous as mentioned above.

The interval-halving method depends on setting upper and lower temperature limits. That is, first, a temperature for which the enthalpy (or entropy) is too high; and second, a temperature for which the enthalpy (or entropy) is too low. The range of much of the JANAF thermochemical data is 298 to 6,000K. These can be chosen as the limits, because if they do not bound the answer, the computer effort is futile anyway.

*This covers a multitude of sins such as no shocking in the nozzle and equal velocities for gas and nongas phases at each point in the flow. Real systems for which this assumption is not valid have what may be referred to as the Type II inefficiency.

The method proceeds as follows: Take the arithmetic mean of the temperature limits $(\overline{T}) = 0.5(T_U + T_L)$ and compute the value of $H(T)$ or $S(T)$ depending on the process. If $H(T)$ is greater than H_0 (or equivalently for S), $\overline{T}$ becomes the new upper limit. Otherwise, it becomes the new lower limit. The process is then repeated. $\overline{T}$ becomes successively a better estimate of the desired temperature, gaining one bit in precision for every iteration. Using the original limits of 298 and 6,000K, about 13 iterations are required to achieve a precision of one degree.

The interval-halving method is the slowest practical approach to the problem. However, it has one overwhelming advantage over other methods; if the answer is contained in the original limits, the method will always converge.

The propellant program combines the two techniques. Temperature bounds are established and modified according to the results of the temperature guesses (a guess too high gives a new upper bound and vice-versa). Guesses are first chosen by the formula for Newton's method. However, they are used only if they do not approach one of the bounds by more than halfway; in this case the halfway point is used.

The program thus uses Newton's method, with an interval-halving "override." The advantages of both methods are obtained. When the curve is fairly linear, the convergence is rapid; when the curve "misbehaves" convergence is at least certain.

ESTIMATION OF NOZZLE DESIGN PARAMETERS

The NWC thermochemical program evaluates theoretical specific impulse by exact methods: enthalpy balance for the combustion process and entropy balance for the expansion process. The state of the fluid immediately after combustion is completed may be designated by the subscript "1" and the state of the gas after isentropic expansion to the exit pressure may be designated by the subscript "2".

The state variables computed during the first process are T_1, V_1 and S_1 given the chamber pressure, P_1, and the propellant heat of formation, H_1. Those computed during the second process are T_2, V_2 and H_2 given the exit pressure, P_2, and entropy, $S_2 = S_1$.

The state of the gas after the expansion may be computed under either a shifting or frozen hypothesis; in the latter case the chamber composition is retained rather than computing new equilibrium conditions at the exit conditions. Obviously, the values of T_2, V_2 and H_2 differ under the two hypotheses, but the design equations presented below (which use these values as input) are identical for both hypotheses.

The computation of optimum impulse assumes that the expansion ratio of the nozzle is optimum; i.e., the value of pressure predicted at the exit by the continuity equation is the same as the given ambient pressure. In this case, impulse is simply evaluated as follows:

$$I_{sp} = \frac{1}{g_{MKS}}\sqrt{\frac{2J(H_1 - H_2)}{m}} \tag{22}$$

where $g_{MKS} = 9.80665$ m/s^2, $J = 4186$ (g-joules)/(kg-calories), $m = 100$ g and H is system enthalpy in calories. (The program does not actually require a 100 g reference mass; it is merely a time-honored convention.)

The questions arise: How does one correct the impulse for conditions other than the chamber and exit pressures given? Also, how does one correct for a nozzle that does not have an optimum expansion ratio? Furthermore, how does one determine design parameters such as the thrust coefficient and the optimum expansion ratio itself?

Two comments can be made immediately: (1) As far as the first question is concerned, there is no better way to determine the correction than rerunning the program at the desired pressure conditions; (2) The gamma equations given in textbooks are inaccurate and misleading, especially when applied to shifting flow and when the conventional definition of gamma is used:

$$\gamma = C_p/C_v \tag{23}$$

However, equations of a gamma form may be used effectively, if the values for gamma are fitted to the exact solution of the state variables yielded by the program.

This approach assumes that the equations of state for enthalpy and entropy may be written:

$$H = H_O + \frac{\gamma_c}{\gamma_c - 1} nRT \tag{24}$$

$$S = S_O = \frac{\gamma_v}{\gamma_v - 1} nR \ln T - nR \ln P \tag{25}$$

where H_O and S_O are arbitrary constants and γ_c and γ_v are the parameters to be fitted.

The perfect gas law, $PV = nRT$, may be substituted into Equations 24 and 25 yielding:

$$H = H_O + \frac{\gamma_c}{\gamma_c - 1} PVL \tag{26}$$

$$S = S_O' + \frac{\gamma_v}{\gamma_v - 1} nR \ln (PV) - nR \ln P \tag{27}$$

where S_O' is a new arbitrary constant, and L = 24.218 calories/liter-atm. is introduced so as to consistently express enthalpy in calories.

The constants γ_c and γ_v are to be determined as that H_2 and V_2 are correctly predicted from H_1 and V_1 by Equations 26 and 27. The solution may be shown to be

$$\frac{\gamma_c}{\gamma_c - 1} = \frac{H_1 - H_2}{P_1V_1 - P_2V_2} \frac{1}{L} \tag{28}$$

$$\gamma_v = \frac{\ln P_2 - \ln P_1}{\ln V_1 - \ln V_2} \tag{29}$$

where H_O and S_O' cancel out. γ_c may be called the *calorimetric gamma* because it predicts the heat content during the expansion. γ_v may be called the *volumetric gamma* because it predicts the changes in volume during the expansion. In fact the familiar relation

$$P_1V_1^{\gamma_v} = P_2V_2^{\gamma_v}$$

may be derived from Equation 29, assuming $\Delta S = 0$. The two gammas will not, in general, be equal, due to nonuniform heat capacity and changes in composition in real systems.

Design calculations may be based on the continuity equation for one-dimensional flow:

$$\dot{m} = k\rho v A \tag{30}$$

where $\dot{m}$ = mass flux (g/s), k = 1,000 (liters/m^3), ρ = density (g/liter), v = velocity (m/s) and A = duct cross-sectional area (m^2).

Equation 30 may be rewritten in terms of state variables.

$$A/\dot{m} = \frac{V/k}{\sqrt{2mJ\ (H_1 - H)}} \tag{31}$$

using the relationships $H_1 - H = 1/2\ m\ v^2$ and $\rho = \frac{m}{v}$.

Equations 26 and 27 may be substituted into this expression giving

$$A/\dot{m} = f(P) = \frac{\sqrt{\frac{P_1 V_1}{m}\ \frac{\gamma_c}{\gamma_c - 1}}}{P_1 k \sqrt{2\ L\ J}} \cdot \frac{\left(\frac{P}{P_1}\right)^{-1/\gamma_v}}{\sqrt{1 - \left(\frac{P}{P_1}\right)^{(\gamma_v - 1)/\gamma_v}}} \tag{32}$$

The pressure at the nozzle throat is found by minimizing this expression with respect to P. The solution is

$$P^* = P_1 \left(\frac{2}{\gamma_v + 1}\right)^{\gamma_v/(\gamma_v - 1)} \tag{33}$$

The throat area for unit mass flow is found by substituting P^* back into Equation 32.

$$A^*/\dot{m} = f(P^*) \tag{34}$$

The optimum expansion ratio for the given exit pressure may now be found

$$(A/A^*)\text{opt} = f(P_2)/f(P^*) \tag{35}$$

If the nozzle expansion ratio is not optimum, then the true exit pressure (P_2') is not the same as the given exit pressure (P_2). P_2' may be found implicitly from the given value of the expansion ratio.

$$(A/A^*)\ \text{given} = f(P_2')/f(P^*) \tag{36}$$

The energy of propulsion is then given by:

$$\Delta H = \frac{\gamma_c}{\gamma_c - 1}\ (LP_1V_1)\left[1 - \left(\frac{P_2'}{P_1}\right)^{(\gamma_v - 1)/\gamma_v}\right] \tag{37}$$

(In the special (optimum) case where $P_2' = P_2$, then $H = H_1 - H_2$.)

In both optimum and nonoptimum cases, the specific impulse is given by

$$I_{sp} = \frac{1}{g_{MKS}}\sqrt{\frac{2J\Delta H}{m}} + JKLf(P_2')\ (P_2' - P_2) \tag{38}$$

The vacuum specific impulse follows easily:

$$(I_{sp})_{\text{vacuum}} = \frac{1}{g_{MKS}}\sqrt{\frac{2J\Delta H}{m}} + JKLf(P_2')\ P_2' \tag{39}$$

Finally, the thrust coefficient and the characteristic velocities are found by conventional relationships.

$$C_f = g_{MKS}\, I_{sp} \Big/ \left[JKLf(P^*)\, P_1\right] \tag{40}$$

$$C^* = g_{FPS}\, I_{sp} \Big/ Cf \tag{41}$$

where $g_{FPS} = 32.16$ ft/s^2.

The program currently outputs $(I_{sp})_{\text{opt}}$, γ_p, (A/A), and C_f under both frozen and shifting hypotheses. Corrections for nonoptimum expansion may be obtained under one of the program options.

The program was modified in 1965 so that the computation of γ_c and γ_p is applied to several regimes. These are separated at points where condensed phases appear and disappear from the system. The values of γ_c and γ_p vary from regime to regime. Each regime is scrutinized for minimum throat area. If more than one occurs, the smallest is the one chosen.

BOOST VELOCITY

The formula for boost velocity of an idealized missile (one free of gravity and drag) is

$$\Delta U = (I_{sp})\ g\ \ell n\ \left(1 + \frac{\rho}{\rho^*}\right)$$

where the switch density, ρ^*, is given by

$$\rho^* = \frac{\text{Mass of missile} - \text{Mass of propellant}}{\text{Volume of propellant}} \tag{42}$$

and ρ is the density of the propellant.

We use lb-mass/in^3 to measure ρ and lb-mass/ft^3 to measure ρ^*, as input to the computer, in abject submission to the illogical common usage. The units are made the same before computing the ratio.

Appendix A

INPUT INSTRUCTIONS FOR THE PROPELLANT EVALUATION PROGRAM (PEP)

The instructions below assume that one is making a batch run and that he has already produced the library tape or file described under PEP Auxiliary Program (Appendix G). It does not describe the optional input of ingredients by serial number; that is described under Automated Input of Ingredient Data (Appendix F). The latter option works for both batch and teletype runs.

The input deck for the equilibrium program consists simply of three groups of cards: (1) the control card, (2) the ingredient composition card(s), and (3) the pressure and weight ratio card(s).

The first 19 columns of the control card contain option switches. Their functions are summarized in Table A-1 at the end of this appendix.

In columns 21 through 26 of the control card appear the first six letters of the name of the person running the problem. Ending in column 30 is the number (not to exceed 10) of propellant ingredients; this number must agree with the number of ingredient composition cards that are to follow the control card (punch no decimal point). Ending in column 40 is the number of runs to be made on that system of ingredients. This number must agree with the number of pressure and weight ratio cards that are to follow the ingredient cards (again, punch no decimal point).

The format of the ingredient composition card is as follows:

Column 1-30	Name of ingredient (alphanumeric)
Column 31-33	Number of atoms of first element in compound (punch no decimal)
Column 34-35	Symbol of first element (left adjust)
Column 36-38	Number of atoms of second element in compound
Column 39-40	Symbol of second element and so on as needed up to six elements and column 60.
Column 63-67	Heat of formation of compound in calories per gram (right adjust with no decimal point)
Column 69-73	Density of compound in pounds per cubic inch (punch decimal point)

This last item may be omitted if boost velocities and density-impulse are not required.

Examples of ingredient composition cards follow:

AMMONIUM DICHROMATE 8H 2N 7O 2CR -1688 .0776

It is possible to introduce arbitrary multipliers into the composition; thus the following is equivalent to the example above:

AMMONIUM DICHROMATE 16H 4N 14O 4CR -1688 .0776

Mixtures may also be entered as single ingredients as follows:

AIR (DRY AT SEA LEVEL) 835N 224O 5AR 0000

The pressure and weight ratio cards each consist of 12 six-column fields. The first field contains the chamber pressure, and the second contains the exhaust pressure. Following these are consecutive weight ratios for the propellant ingredients in the same order in which they appear in the ingredient composition cards. There are, of course, as many cards as there are ingredients. The weights normally are chosen to add up to 100 g, although this is not required. *Decimal points must be punched in all fields used on the pressure and weight ratio cards.*

A complete sample input deck for a well-known hybrid system is listed after Table A-1 Table A-1 contains necessary information that should be studied before using the program.

TABLE A-1. Program Options.

Option no.	Type	Function performed
1	1	Deletes exit calculations
2	1	Includes ionic species in the calculations
3	1	Deletes boost velocities and three pages of nozzle design data
4	1	Inputs pressures in psi instead of atmospheres
5	1	Increases precision of species concentrations one order of magnitude
5	2 or higher	Increases precision even further
6	1	Inputs an extra identification card
7	1	Inputs a pressure-temperature point instead of chamber and exhaust pressures. This allows a P-T-H-S chart to be developed
8	1	Outputs a list of all combustion species considered
9	1	Allows serial number input for ingredients
10	1	Allows modification of H and ρ data
		Option 11-15 are used only for debugging
11	1	Prints out thermo data computed at every temperature guess
12	1	Prints out the first guess of the composition
13	1	Prints out compositions every fourth iteration
14	1	Prints out the log of the equilibrium constants at every temperature guess
15	1	Outputs a code that indicates the classification the program has applied to various species at each iteration
16-19	Leave Blank	For internal use

```
-RUN 419051.1320018AOB5G.4535419.05.75/0     CRUISE
-ADD PEP*RUN.
0011000000            CRUISE   2          9
SULPHUR                                 1S                                  +0000 .0474
MOLASSES                                22H   12C   110                     -1550 .0574
 1000.   14.7    10.    90.
-FIN
```

Appendix B

PEP TELETYPE USAGE
(Pertains mainly to NWC users)

First obtain a user number for yourself, an identification number for your teletype (TTY), and a job order number for the use of the people in Code 3132. Call Ext. 3019 for a UNIVAC 1110 user number, and call Daryl Vaughn at ext. 3561 for the teletype identification number, if it is not already pasted to your teletype.

Approach the teletype and dial 7 (120 cps), 6 (.)0 cps), or 5 (10 cps). It should ring once and give a 1,000-cps beep. Type in the teletype identification upon coupling. A secret password is now required at this point (call ext. 3019 for information).

The RUN card is typed next. It starts with @RUN followed by one or more spaces. Then, on the same line, type uuuTTY, mmmmmmmmmm9G, ccccuuu, t, where uuu is your user number, mmmmmmmm is your job order number, cccc is your NWC organizational code, and t is a time estimate in minutes. The TTY and 9G are typed as shown.

After the computer prints out the date, type in @ADD PEP*RUN. exactly as shown. (Do not forget the period.)

The computer will now mumble for 10 or more lines, and then you will be greeted by the PEP program. The program will prompt you for an input and provide a typing guide. The first inputted line contains the options, the name of the user, the number of ingredients, and the number of runs to be performed on that set of ingredients. Type the options under the option number.

Ingredient information may now be entered by serial number. Obtain a list from Code 3245, and send any updates for the list you wish to add. Enter the serial numbers in the order you wish and type them consecutively so they end under the "V's" of the typing guide. (They a thus right adjusted in five-column fields.)

The program will next prompt you for the chamber pressure, the exit pressure, and the weight ratios. The weight ratios are in the same order as the ingredients. Always type the decimal point and remain inside the fields. The end of each field is indicated by a "V" in the typing guide. (Actually the guide stops short of the 12 fields that are possible.) The number of ingredients is limited to 10.

If you wish to start over, hit a carriage return instead of the input discussed above.

Terminate the run by typing @@X TIO and then @FIN instead of the prompted input. After the computer prints out execution time, type @@TERM to sign off.

A "control Z" deletes the previous character (but defeats the typing guide).

A "control X" typed before a carriage return deletes the current line and allows you to start over.

A run may be aborted by hitting the "break" key (on some teletypes this must be followed by hitting a "break release" button, which turns on after you have hit the "break" key). The computer

types INTERRUPT LAST LINE and returns. Type @@X TIO and hit carriage return. The run eventually stops.

If a run is deliberately or accidentally aborted, type @XQT CRUISE*QAME to restart the program, instead of @ADD PEP*RUN; it saves time and money.

To save more money, try the following:

1. Delete the long output (option 3), if you do not need it.
2. Punch the information on cards and submit a batch run.
3. If you do not mind the longer turnaround time, submit a batch run with an "N" (night run) option.

Appendix C

COMMENTS ON THE PEP OUTPUT

The program output deliberately has been made concise so that a great deal of information may appear on a single page of a report. However, the conciseness requires that some explanations be given to the uninitiated.

The first line contains the user's name, the date, and the precise time of day. This information is repeated on successive pages so that, if the pages are separated, they are uniquely identified.

The input ingredients are printed next, so that the input may be checked.

The ingredient weights are printed next, and the total system weight follows the individual weights. The total system weight is generally chosen by the user to be 100 g, but whatever the user chooses, the value is important to other outputs described below.

The gram-atom amounts for each chemical element are next. These are based on the given system weight.

The chamber conditions are then printed out with headings. The enthalpy has units of kilocalories per system weight, and the entropy has units of calories/K per system weight. CP/CV is the ratio of specific heats, and GAS identifies the number of moles of gas produced per system weight. Effective molecular weight is obtained by dividing GAS into system weight. Note that although nongases are not included in this computation this is the proper molecular weight to use in gas dynamic equations. The quantity RT/V is equal to the variable designated A in the text and may be expressed as

$$A = \frac{R\ (0.08205\ \ell\text{-atm/mole/K})\ T\ (K)}{V(\text{system volume in liters})}$$

The chamber composition follows in units of moles per system weight. If one prefers to obtain partial pressures in atmospheres, multiply each composition by RT/V printed above.

The exhaust plane results follow, in the same format and units as the chamber results just described.

Three lines of performance results appear next. The first contains headings; the second contains the results for a frozen flow (no chemical reactions) through the nozzle; and the third contains results for a shifting flow (reactions in equilibrium) through the nozzle. Impulse is in the units of seconds and is the same in engineering and metric units. Unfortunately, the SI people introduced confusion where none previously existed by changing the definition of impulse to what was previously called the theoretical exhaust velocity. Therefore, to obtain the official SI impulse, multiply the value outputted by 9.806 m/sec.

The next number (IS EX) is the isentropic exponent, which is the number, γ_p such that

$$PV^{\gamma_p} = \text{constant}$$

for isentropic flow near the nozzle throat. The values of IS EX and CP/CV do not agree, because the gas is not perfect.

The variables T* and P* are throat temperature (in K) and pressure (in atmospheres), respectively. The variable CF is the nozzle thrust coefficient. Those who regard characteristic velocity, C*, as a meaningful number may obtain it by the relation

$$C^* = 32.17\ ISP/CF$$

The variable, ISP*, is the vacuum impulse to be obtained from a sonic nozzle. That term is used in airbreathing propulsion work. The optimum expansion ratio (OPT EX) is the ratio of the nozzle exit area to nozzle throat area at which exit pressure equals ambient pressure. The density impulse is labeled D-ISP, and the exit plane temperature is in K.

Appearing just before the exit temperature (EX T) is A*M., which stands for $A^*/\dot{M}$. This is the ratio of nozzle throat area to mass flow rate expressed as in^2-sec/lb.

Optional output includes boost velocities. These are shown in number pairs: the first is the switch density (see text), and the second is the velocity in feet/second. Inputted densities follow in pounds/in^3. The next output shows the performance of the propellant through nozzles with expansion ratios of 1 to 100. These include three kinds of impulse: optimum (ambient pressure = exit pressure), vacuum (zero exit pressure), and sea level (exit pressure = 1 atmosphere). Units are given in SI units as well as the older English units. Note that all impulses need to be corrected for nozzle half angle.

A final output shows the computer CPU time consumed by the calculations.

```
CRUISE  09/15/78     09:43:43          DH   COMPOSITION

 SULFUR                                 0    1S
 MOLASSES                            -1550   22H   12C   11O

INGRED. WTS.&TOTAL/ GRAM ATOMS/ CHAMBER/ EXHAUST RESULTS/ PERFORMANCE

 10.00000   90.00000 100.00000

 5.784264 H     3.155053 C     2.092132 O      .311857 S

 T(K)  T(F)  P(ATM)   P(PSI) ENTHALPY  ENTROPY   CP/CV    GAS    PT/V
 850. 1071.   68.02  1000.00  -139.50   169.12  1.1664  3.169  21.465

  1.75964 CS        1.26292 H2O         .79298 CO2         .55919 CH4
   .30977 H2S        .20107 H2          .04116 CO          .00209 CSO
  1.25-06 CS2

 T(K)  T(F)  P(ATM)   P(PSI) ENTHALPY  ENTROPY   CP/CV    GAS    PT/V
 501.  442.    1.00    14.70  -156.92   169.12  1.2045  3.059   .327

  2.15012 CS        1.72024 H2O         .56569 CO2         .41894 CH4
   .31181 H2S        .02221 H2          .00005 CO          .00004 CSO


IMPULSE  IS EX     T*      P*      CF    ISP*  OPT EX  D-ISP    A*M.    EX T

 120.2  1.1936   775.  38.48  1.625            8.98      .0  .07401   429.
 123.1  1.1483   797.  39.14  1.628   93.4     9.67      .0  .07563   501.

INGRED. DENSITIES ARE
  .0000    .0000

(CPU  1.79SECS.)
```

Appendix D

BRIEF DESCRIPTIONS OF PEP SUBROUTINES

In the summary below the first item to appear is the subroutine name. Then appears a letter code in parentheses to explain the usage of the subroutine. The meanings of the letters are as follows:

(M) Main program
(I) Input routine
(O) Output routine
(E) Routine directly involved in equilibrium calculations
(P) Routines that evaluate performance
(U) Utility routine

Following the letter code appears the name of the calling subroutine(s) in square brackets. Finaliy a brief description appears.

A summary of the PEP subroutines follows:

ADJUST (E) [DEFIOJ] Correct errors in gram-atom balance that arise due to truncation errors.
BOOST (P,O) [DESIGN] Computes and outputs boost velocities.
*DATE (U) Calendar date routine.
DEFIOJ (E) [EQUIL] Computes optimal basis.
DESIGN (P,O) [PEP] Computes and outputs performance parameters.
DESNOZ (O) [PEP] Outputs nozzle performance.
EQUIL (E) [HBAL,SBAL] Computes composition for a pressure-temperature point.
FIXBAS (E) [EQUIL] Fixes basis to compensate for phase changes that occur due to temperature change.
GIBBS (D) [EQUIL] Computes enthalpy, entropy, and Gibbs free energies for all species.
GUESS (E) [PEP] Computes initial guess of composition.
HBAL (E) [PEP] Computes constant pressure combustion (P,H point).
IPHASE (P) [DESIGN] Characterizes and locates phase changes.
LINDEP (E) [DEFIOJ] Establishes linear independence of basis.
*LKCLKS (U) [PUTIN] Looks at system clock.
ONED (P) [DESIGN] One-dimensional flow calculations.
OUT (O) [PEP] Outputs temperatures and composition.
PEP (M) Main program puts everything together.
PUTIN (I) [PEP] Main input routine.
RANK (U) Sorts an array into decreasing order of size.
REACT (E) [EQUIL] Computes stoichiometric coefficients and equilibrium constants.
SBAL (P) [PEP] Computes isentropic exhaust state (i.e., a P,S point).

*Nonessential system utility subroutines.

SEARCH (I) [PUTIN] Searches combustion data for pertinent species.
*SETCLK (U) Sets the system clock to zero.
SETUP (E) Preliminary analysis of equilibrium situation, computes maximum and minimum shifts in concentration so that negative concentrations do not occur.
SLITE,SLITET (U) Through this routine the program seeks to turn off simulated lights to obtain:
LITE(1) off--optimum basis
LITE(2) off--linear independence in basis
LITE(3) off--temperature convergence
LITE(4) off--composition convergence
STOICH (E) [PUTIN] Preliminary analysis of elementary composition.
TABLO (E) [TWITCH] Updates optimal basis by the tableau method of linear programming.
TAPEB (I) [SEARCH] Input buffer for combustion data.
THERMO (E) [EQUIL] Computes system enthalpy and entropy.
*TOFDAY (U) Time of day.
TSALT (P) [TSBAL] Computes a T,S point by slow, but reliable method when TSBAL fails.
TSBAL (P) Fast equilibrium computation for specified temperature and entropy (T,S); occasionally fails to converge.
TWID (E) [TWITCH] Computes equilibrium relation for TWITCH to modify.
TWITCH (E) [EQUIL,TSBAL] Main equilibrium subroutine. This is flow-charted below.

*Nonessential system utility subroutines.

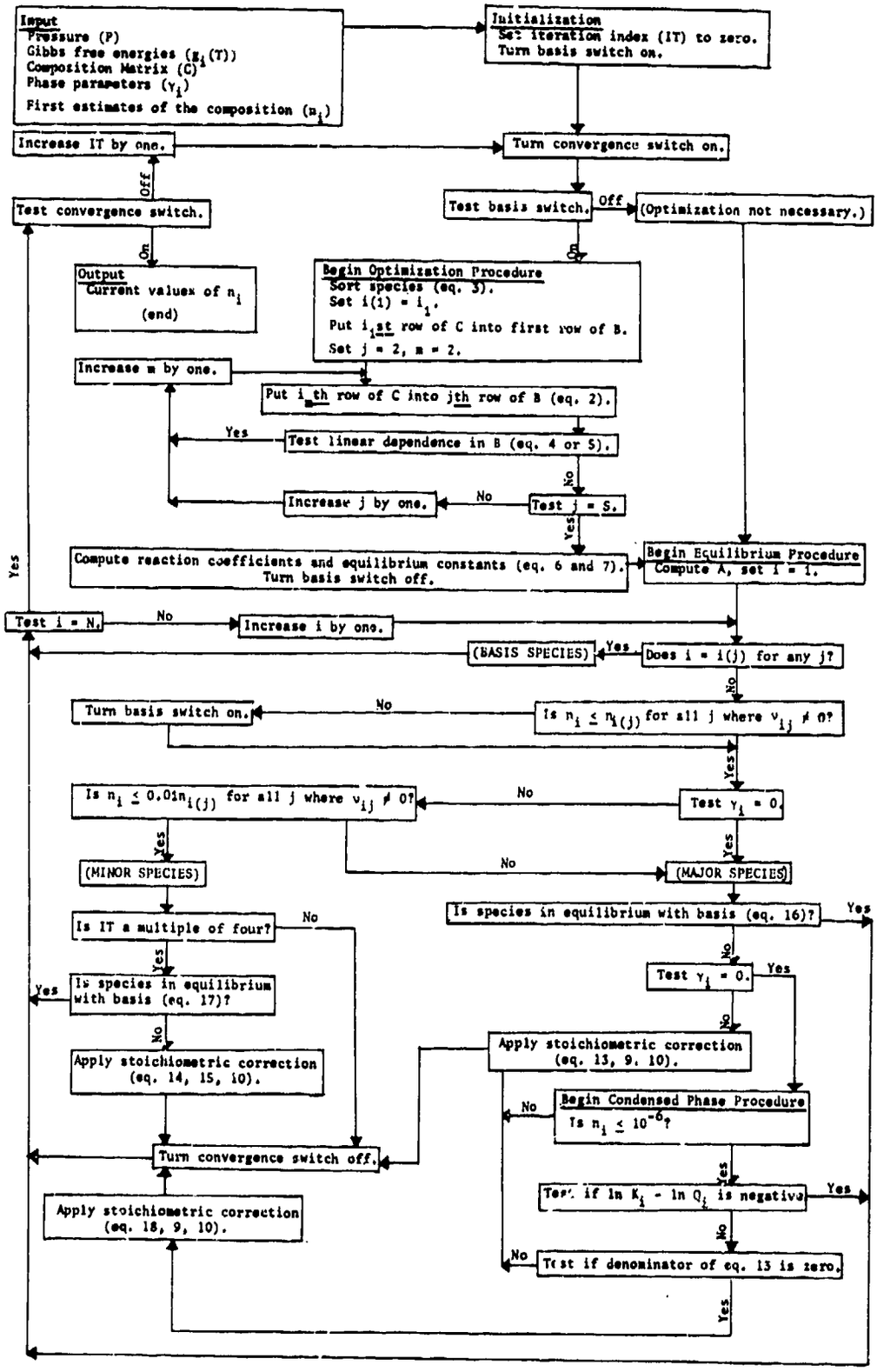

FIGURE D-1. Flow Chart for Computation Procedures.

Appendix E

IDENTIFICATION OF VARIABLES IN COMMON BLOCKS

The following information is provided for those who wish to dig into the equilibrium program.

BLANK COMMON

A	Basis matrix
KR	Option block
AMAT	Ingredient composition matrix
JAT	Atomic numbers
ASPEC	Element names (field data)
IN	Number of ingredients
IS	Number of elements
FIE, IE	Ingredient composition
ALP	Gram-atom amounts (α)
W27	System weight
N	Number of combustion species
BLOK	Ingredient names (field data)
DH	Ingredient heats of formation
RHO	Ingredient densities
ISERI	Output identification (field data)
WATE	Ingredient weights
W1(4)	System heat of formation
W1(5)	Chamber pressure
W1(6)	Exhaust pressure
W43	Density
IG	Number of gaseous combustion species
NP	N + 1
VNT	Combustion species concentrations
W47	Temporary
NAME	Temporary
SER	Temporary
FLOOR	Lower limit of concentrations

COMMON/IBRIUM

TL	Lower temperature limits for species data
TU	Upper temperature limits
W3	Molecular weights of species
VNU	Reaction coefficient matrix (ν_{ij})
QA	Temporary variable
TAU	Temporary variable
H	Species enthalpy
SD	Species entropy
Y	Species heat capacity
JC	Iteration index
IR	Storage area for sorting
DMU	Species Gibbs free energies (u_j)
VLNK	Natural log of equilibrium constants
IOJ	Indices for basis species (i(j))
RA	Constant terms for species c_p (L_1)
RB	T term for species c_p (L_2)
RC	T^2 term for species c_p (L_3)
RD	T^3 term for species c_p (L_4)
RE	T^{-2} term for species c_p (L_5)
RF	Reference enthalpies (L_6)
CH	Reference entropies (L_7)
JM	Temporary variable
W48	Temporary variable
CP	System heat capacity
FN	Number of moles of gas in system
C	Species composition matrix
SPECIE	Names of species (field data)
LL	Vectro to keep track of certain computational data concerning combustion species

COMMON/SCRATC/

HN	Temporary storage for compositions. This is used to analyze splits between the liquid and solid phase of a species.
PLOT	Temporary storage for nozzle design results.

COMMON/MOON/

TSTEST	Convergence test for T-S point.

Appendix F

AUTOMATED INPUT OF INGREDIENT DATA

The program (PEPLIB) appears below with data. It allows a user to enter ingredient data, if he is lucky enough to find it on the list, by the serial number that appears to the right. If option 9 is employed, the ingredient serial numbers are punched on a single card following the option card in format (10I5). PEPLIB creates a tape or file which is given label "11" by both PEP and PEPLIB.

The program date is the compilation of propellant ingredient data as of 10 May 1978. It contains many corrections and additions to previous lists.

It is not convenient to the users to reassign serial numbers once assigned to an ingredient. Therefore, note that the oldest data is in alphabetical order. Following that is a supplementary list that is also in alphabetical order. Following that is another list of several dozen ingredients, which are in the order received. Finally, there are two more supplementary lists, one of which is data received from Ed Barooty at NSWC, Indian Head, MD. This is heat of combustion data and is in alphabetical order.

Chemical ingredient names are mostly generic to avoid confusion. Since these are sometimes long, they are sometimes continued on the following line. The proper serial number in that case is on the line which contains the composition.

Program With Truncated Input

```
-ASG,AX CRUISE*PEPLIB//21734
-USE 11,CRUISE*PEPLIB
-FOR,IS   LIBPRO,LIBPRO/A
      DIMENSION A(20), B(2)
      WRITE (6,4)
    4 FORMAT (-1-)
      REWIND 11
      DO 9  J=1,9999
      READ (5,1,ERR=10,END=11)(A(I),I=1,13)
C     1 FORMAT (10A6,2X,A5,1X,A5,1X,A6)
    1 FORMAT (10A6, 1X, F6.0, 1X, A5, 1X, A6)
      ENCODE(19,8) A(11)
   19 FORMAT (F6.0)
      A(11)=B(1)
      WRITE (11,5)(A(I),I=1,12)
    5 FORMAT (10A6,A5,1X,A5,1H))
C     2 FORMAT (12A6,A1,I7)
      JJ=J-1
    9 WRITE (6,3)(A(I),I=1,12),JJ
    3 FORMAT (- -10A6,2X,A5,1X,A5,I7)
      GO TO 11
   10 READ (30,20)(A(L),L=1,14)
      WRITE ( 6,20)(A(L),L=1,14)
   20 FORMAT(13A6,A2)
   11 END FILE 11
      CALL EXIT
      END
-XQT
```

```
1EA-5-85 (VICTOR)                 378H 243C 102N  860 205F          -0538 1.463    615
2 NITRO DIPHENYL AMINE             10H  12C   2O   2N             +0135 .0535     59
100DER321/43DEH14                 810H 596C  22N 1080             -0661
2 NITRO DIPHENYL AMINE             10H  12C   2O   2N             +0135 .0535     359
2-TDMECLO4 (INFO 635P)              3C   7H   1CL  6F   4N  5O   -0345 .0650  $4001
2-TDMEHCL (INFO 631C)               3C   7H   1CL  6F   4N  1O   -0448 .0650  $4002
8C8H18F10N6O (FAPEMON)              8C   8H   18F  10N  6O        -0273 .0000  *5003
8C8H18F10N6O (FAPEMON)              8C   8H   18F  10N  6O        -0240 .0000  G5004
9C14H12F6N3O (TVOPA)                9C  14H   12F   6N  3O        -0385 .0000  G5005
9C14H12F6N3O(TVOPA)                 9C  14H   12F   6N  3O        -0430 .0554  *5006
ACETAMIDE                           2C   5H   1O   1N            -1310 .0360
ACETYL TRIETHYL CITRATE            22H  14C   8O                 -1257 .0408    008
ACETYLENE                           2C   2H                      +1846 .0263  $5009
ACETYLENE                           2C   2H                      +1892 .0220  *5010
ACETYLENE (GASEOUS)*                2H   2C                      +2081        G 011
ACRYLIC ACID          -HC-          4H   3C   2O                 -1282 .0384  * 012
ACRYLIC NITRILE                     3C   3H   1N                  0682 .0000  *1013
ADIPIC ACID          6C  10H   4O                                 -1480
AIR (DRY AT SEA LEVEL)            835N 2240  5AR                 +0000
AIR  (500K OR 900R)               835N 2240  5AR                 +0049
AIR  (1000R OR 555.56K)           835N 2240  5AR                 +0063
AIR  (750K OR 1350R)              835N 2240  5AR                 +0113
AIR  (1500R OR 833.33K)           835N 2240  5AR                 +0135
AIR  (1000K OR 1800R)K)           835N 2240  5AR                 +0180
AIR  (2000R OR 1111.1K)           835N 2240  5AR                 +0201
AIR  (1250K OR 2250R)K)           835N 2240  5AR                 +0249
```

Program Output

								0	0
1EA-5-85 (VICTOR)	37EH	243C	102N	86O	2O5F		-538	1.463	1
2 NITRO DIPHENYL AMINE	10H	12C	2O	2N			135	.0535	2
10CDER321/43B EH14	81OH	5Y6C	22N	1O8O			-661		3
2 NITRO DIPHENYL AMINE	10H	12C	2O	2N			135	.0535	4
2'TDMECLO4 (INFO 635P)	3C	7H	1CL	6F	4N	5O	-345	.0650	5
2'TDMEHCL (INFO 631C)	3C	7H	1CL	6F	4N	1O	-448	.0650	6
C6H16F1ON6O (FAPEMON)	3C	8H	16F	1ON	6O		-273	.0000	7
8C8H16F1ON6O (FAPEMON)	8C	8H	16F	1ON	6O		-240	.0000	8
9C14H12FON3O (TVOPA)	9C	14H	12F	6N	3O		-385	.0000	9
9C14H12FON3O(TVOPA)	9C	14H	12F	6N	3O		-430	.0554	10
ACETAMIDE	2C	5H	1O	1N			-1310	.0360	11
ACETYL TRIETHYL CITRATE	22H	14C	8O				-1257	.0408	12
ACETYLENE	2C	2H					1846	.0263	13
ACETYLENE	2C	2H					1892	.0220	14
ACETYLENE (GASEOUS)*	2H	2C					2081		15
ACRYLIC ACID -HC-	4H	3C	2O				-1282	.0384	16
ACRYLIC NITRILE	3C	3H	1N				682	.0000	17
ADIPIC ACID 6C 10H	4O						-1460		18
AIR (DRY AT SEA LEVEL)	835N	2240	5AR				0		19
AIR (50CK OR 90CR)	835N	2240	5AR				49		20
AIR (100OR OR 555.56K)	835N	2240	5AR				63		21
AIR (75CK OR 135OR)	835N	2240	5AR				113		22
AIR (125OR OR 833.33K)	835N	2240	5AR				135		23
AIR (100CK OR 1800R)K)	835N	2240	5AR				180		24
AIR (200,R OR 1111.1K)	835N	2240	5AR				201		25
AIR (125OK OR 2250R)K)	835N	2240	5AR				249		26
ALUMINUM (PURE CRYSTALINE)	1AL						0	.0976	27
ALUMINUM (PURE CRYSTALINE)	1AL						0	.0976	28
ALUMINUM DIBORIDE	2B	1AL					-1632	.1152	29
ALUMINUM BERYLLIUM (ALLOY)	1BE	1AL					0	.0874	30
ALUMINUM BERYLLIUM (ALLOY)	3BE	1AL					0	.0795	31
ALUMINUM BORIDE	12B	1AL					-314	.0921	32
ALUMINUM BORON (ALLOY)	12B	1AL					-600	.0978	33
ALUMINUM BOROHYDRIDE	1AL	3B	12H				-301	.0199	34
ALUMINUM BOROHYDRIDE	1AL	3B	12H				-208	. 0	35
ALUMINUM CARBIDE	4AL	3C	-0	-0	-0		-215	.0852	36
ALUMINUM FLOURIDE	3F	1AL					-844		37
ALUMINUM HYDRIDE	1AL	3H					-92	.0516	38
ALUMINUM NITRIDE	1N	1AL					-1407	.1170	39
ALUMINUM (NON-REACTIVE)	1O4						0	.0976	40
ALUMINUM PERCHLORATE	12O	1AL	3CL				-614	.0939	41
ALUMINUMBOROHYDRIDEDIMETHYLAM	2C	19H	1AL	3B	1N		-468	.0265	42
AMINOXYLENE (XYLIDENE)	11H	8C	1N				-65		43
AMINO TETROZOLE	3H	1C	5N				585	.0595	44
AMINE TERMINATED POLYBUTADIENE	6H	4C					56	.0360	45
AMINO TETROZOLE PERCHLORATE	4H	1C	5N	4O	1CL		204	.0668	46
AMMONIUM ACETATE	2C	7H	2O	1N			-1820	.0422	47
AMMONIUM BICARBONATE	1C	5H	3O	1N			-2580	.0570	48
AMMONIUM CARBONATE	1C	8H	2N	3O			-2340		49
AMMONIUM CHLORIDE	1N	4H	1CL				-1410	.0551	50
AMMONIUM CYANATE	1C	4H	1O	2N			-1245	.0484	51
AMMONIUM FLOURIDE	4H	1N	1F				-3000	.0364	52
AMMONIUM FLOUROSILICATE	2N	8H	1SI	6F			-3530	.0726	53
AMMONIUM FORMATE	1C	5H	2O	1N			-2105	.0462	54
AMMONIUM GLYCOLLATE	2C	7H	3O	1N			-1410		55
AMMONIUM GLYOXALLATE	2C	7H	4O	1N			-2100		56
AMMONIUM IODIDE	4H	1N	1I				-336		57
AMMONIUM NITRATE	4H	2N	3O				-1090	.0623	58
AMMONIUM NITRATE	4H	2N	3O				-1090	.0623	59
AMMONIUM OXALATE	8H	2C	2N	4O			-2160	.0542	60
AMMONIUM OXALATE	2C	8H	4O	2N			-2160		61
AMMONIUM OXALATE (HYDRATED)	2C	10H	5O	1N			-2400	.0542	62

AMMONIUM PERCHLORATE (AP)	1CL	4H	1N	4O			-602	.0704	63
AMMONIA TRIBORANE	3B	10H	1N				-867	.0000	64
AMMONIA	3H	1N					-1004	.0244	65
AMMONIA (GASEOUS)*	3H	1N					-649		66
AMMONIATED ALUMINUM IODIDE	1AL	3I	9N	27H	-0		-676	.0000	67
AMMONIATED ALUMINUM IODIDE	1AL	3I	13N	39H	-0		-722	.0000	68
AMMONIATED ALUMINUM IODIDE	1AL	3I	20N	60H	-0		-782	.0000	69
AMMONIATED ALUMINUM IODIDE	1AL	3I	6N	18H	-0		-622	.0000	70
AMMONIATED ALUMINUM IODIDE	1AL	3I	1N	3H	-0		-282	.0000	71
AMMONIATED ALUMINUM IODIDE	1AL	3I	3N	9H	-0		-454	.0000	72
AMMONIATED ALUMINUM IODIDE	1AL	3I	5N	15H	-0		-592	.0000	73
AMMONIATED ALUMINUM IODIDE	1AL	3I	7N	21H	-0		-645	.0000	74
AMMONIATED BERYLLIUM IODIDE	1BE	2I	4N	12H	-0		-642	.0000	75
AMMONIATED BERYLLIUM IODIDE	1BE	2I	6N	18H	-0		-690	.0000	76
AMMONIATED BERYLLIUM IODIDE	1BE	2I	13N	39H	-0		-792	.0000	77
AMMONIATED CALCIUM IODIDE	1CA	2I	1N	3H	-0		-507	.0000	78
AMMONIATED CALCIUM IODIDE	1CA	2I	2N	6H	-0		-570	.0000	79
AMMONIATED CALCIUM IODIDE	1CA	2I	6N	18H	-0		-720	.0000	80
AMMONIATED CALCIUM IODIDE	1CA	2I	8N	24H	-0		-735	.0000	81
AMMONIATED COPPER NITRATE	1CU	4N	6O	6H	-0		-630	.0000	82
AMMONIATED COPPER NITRATE	1CU	6N	6O	12H	-0		-769	.0000	83
AMMONIATED COPPER NITRATE	1CU	8N	6O	18H	-0		-822	.0000	84
AMMONIATED LITHIUM IODIDE	1LI	1I	1N	3H	-0		-608	.0000	85
AMMONIATED LITHIUM IODIDE	1LI	1I	2N	6H	-0		-691	.0000	86
AMMONIATED LITHIUM IODIDE	1LI	1I	3N	9H	-0		-751	.0000	87
AMMONIATED LITHIUM IODIDE	1LI	1I	4N	12H	-0		-799	.0000	88
AMMONIATED LITHIUM IODIDE	1LI	1I	5N	15H	-0		-825	.0000	89
AMMONIATED LITHIUM IODIDE	2LI	2I	11N	33H	-0		-417	.0000	90
AMMONIATED LITHIUM IODIDE	1LI	1I	7N	21H	-0		-857	.0000	91
AMMONIATED MAGNESIUM IODIDE	1MG	2I	2N	6H	-0		-500	.0000	92
AMMONIUM ALUMINUM PERCHLORATE	12H	3N	24O	1AL	3CL		-514	.0756	93
AMMONIUM AZIDE	4H	4N					452	. 486	94
AMMONIUM AZIDE	4H	4N					452	.0486	95
AMMONIUM BOROFLUORIDE	4H	1B	1N	4F			-2860	.0668	96
AMMONIUM BROMIDE	4H	1N	1BR				-659	.0878	97
AMMONIUM CYANIDE	2N	4H	1C	-0	-0		0	.0000	98
AMMONIUM DICHROMATE*	8H	2N	7O	2CR			-1688	.0776	99
AMMONIUM DICYANAMIDE	2C	4H	4N				121	.0000	100
AMMONIUM FLOURIDE	4H	1N	1F				-1287		101
AMMONIUM FORMATE	5H	1C	1N	2O			-2108		102
AMMONIUM IODIDE	4H	1N	1I				-334		103
AMMONIUM PERIODATE	4H	1N	4O	1I			-360	.1270	104
AMMONIUM PERCHLORATE	340H	340O	85N	85CL			-590	.0704	105
AMMONIUM SULPHATE	8H	2N	4O	1S			-2133	.0643	106
AMYL FERROCENE	20H	15C	1FE				-81	.0422	107
ANILINE	7H	6C	1N				79	.0367	108
ARGON	1AR	-0			0		0	.0644	109
ASYROGELL	30H	15O	1O	1AL			-436	.0540	110
AZO*BIS*ISOBUTYRONITRILE*2,2	8C	12H	4N				333	.0000	111
BARIUM CHROMATE	1CR	4O					-1347		112
BARIUM NITRATE *	2N	6O	1BA				-907	.1170	113
BARIUM PEROXIDE	1BA	2O	-0	-0	-0		-889	.1791	114
BASIC LEAD CARBONATE	3PB	2C	8O	2H			?		115
BENZENE	6H	6C					143	.0317	116
BERYLLIUM BOROHYDRIDE	2B	1BE	8H				-666	.0218	117
BERYLLIUM HYDRIDE	1BE	2H					-399	.0000	118
BERYLLIUM NITRIDE	3BE	2N	-0	-0	-0		-2464	.0000	119
BERYLLIUM (NON-REACTIVE)	1O2						0	.0668	120
BERYLLIUM (PURE CRYSTALINE)	1BE						0	.0668	121
BIS TRIAMINOGUANIDINIUMDECABOR	2C	28H	10B	12N			180	.0000	122
BISDIFLUOROAMINOHEPTANE	7C	14H	4F	2N			-220	.0426	123
BIS(CMETHYLHYDRAZINO)DECABORA	4C	26H	10B	6N			100	.0404	124
BIS(DIFLUOROAMINO)BUTANE*2,3	4C	8H	4F	2N			-353	.0437	125
BIS(DIFLUOROAMINO)DIFLUOROMETH	1C	6F	2N				-698	.0000	126
BIS(DIFLUOROAMINO)METHYLPENTAN	6C	12H	4F	2N			-309	.0000	127
BIS(DINITROFLUORETHYL)FORMAL	5C	6H	2F	4N	10O		-559	.0576	128

BIS(DINITROPROPYL)ACETAL BDNPA	8C	14H	4N	100			-470	.0465	129
BIS(DINITROPROPYL)FORMAL BDNPF	7C	12H	4N	100			-475	.0516	130
BIS(FLUOROXY)DIFLUOROMETHANE	1C	4F	2O				-1122	.0000	131
BIS(TRINITROETHYL)NITRAMINE	4C	4H	5N	140			13	.0 08	132
BIS(DIFLUOROAMINO)BUTANE-2,3	4C	8H	4F	2N			-348	.0438	133
BIS(DIFLUOROAMINO)METHYLPENTAN	6C	12H	4F	2N			-363	.0415	134
BIS(DIFLUOROAMINO)OCTANE-2,2	8C	16H	4F	2N			-347	.0397	135
BIS(DINITRO) FLUOROPROPANE	3C	5H	1F	2N	4O		-530	.0000	136
BIS(DINITROPROPYL)ACETAL BDNPA	8C	14H	4N	100			-485	.0491	137
BIS(DINITROPROPYL)FORMAL BDNPF	7C	12H	4N	100			-467	.0511	138
BIS(FLUOROXY)DIFLUOROMETHANE	1C	4F	2O				-1159	.0433	139
BIS(METHYLHYDRAZINO)DECABORANE	2C	24H	10B	4N			-470	.0000	140
BORINE AMMONIATE	1B	6H	1N				-1340	.0264	141
BORON (PURE CRYSTALINE)	1B						0	.0845	142
BORON (AMORPHOUS)	1B						37	.0856	143
BORON CARBIDE	4B	1C					-221	.0905	144
BORON NITRIDE	1B	1N					-2430	.0795	145
BORON SLURRY	553H	861B	252O	450		2AL	-425	.0536	146
BORON OXIDE	2B	3O					-4339	.0656	147
BORON (TRONA)	67B	3O					-359	.0845	148
BROMINE PENTAFLUORIDE	1BR	5F					-627	.0883	149
BROMINE PENTAFLUORIDE	1BR	5F					-586	.0000	150
BROMINE MONOFLUORIDE	1BR	F					-141	.0000	151
BROMINE TRIFLUORIDE	1BR	3F					-530	.1012	152
BROMINE TRIFLUORIDE	1BR	3F					-446	.0000	153
BTNEC	4H	5C	6N	150			-430	.0680	154
BTNEN	4H	4C	8N	140			39	.0704	155
BUTAREZ (PHILLIPS INFO)	519H	347C	8O				-21	.0325	156
BUTANE(2,2-BISDIFLUOROAMINO)	4C	8H	4F	2N			-318	.0000	157
BUTANE(2,3-BISDIFLUOROAMINO)	4C	8H	4F	2N			-348	.0000	158
BUTAREZ (PHILLIPS INFO)	519H	347C	8O				-21	.0325	159
BUTYL SILANE	12H	4C	1SI				357	.0000	160
BUTYLNITRAMINE (NORMAL)	4C	10H	2N	2O			-264	.0385	161
BUTYL RUBBER	8H	4C					-376	.0332	162
CALCIUM BORIDE	519H	347C	8O				-21	.0325	163
CALCIUM CARBIDE	2C	1CA					-234	.0801	164
CALCIUM CARBONATE (CACO3)	1C	3O	1CA				-2895		165
CALCIUM CHLORIDE	2CL	1CA					-1710	.0775	166
CALCIUM FLUORIDE	2F	1CA					-3722	.1149	167
CALCIUM HYDRIDE	2H	1CA					-1092	.0614	168
CALCIUM NITRATE	1CA	2N	6O	-0	-0		-1365	.0852	169
CALCIUM PEROXIDE	1CA	2O	-0	-0	-0		-2185	.0000	170
CALCIUM OXIDE (CAO)	1C	1CA					-2710		171
CANDELILLA WAX	2C	4H					-453	.0325	172
CANDELILLA WAX	2C	4H					-453	.0325	173
CARBON BLACK	1C						0	.0637	174
CARBON DIOXIDE	1C	2O					-2137	.0398	175
CARBON DISULFIDE (WHEW)	1C	2S					276	.0456	176
CARBON MONOXIDE	1C	1O					-943	.5721	177
CARBON (GRAPHITE)	1C						0	.0818	178
CARBON TETRACHLORIDE	1CA	4CL					-216		179
CELLULOSE	6C	10H	5O				-1417	.0458	180
CELLULOSE ACETATE (2)	149H	109C	74O				-1183	.0539	181
CELLULOSE ACETATE (CARBOPOL)	149H	109C	74O				-1079	.0448	182
CELLULOSE DINITRATE	6C	8H	2N	9O			-7144	.0599	183
CELLULOSE TRINITRATE	6C	7H	3N	11O			-524	.0599	184
CELOGEN	2C	4H	2O	4N			-1001		185
CERIUM	1CE	-0	-0	-0	-0		0	.2419	186
CERIUM NITRIDE	1CE	1N	-0	-0	-0		-508	.0000	187
CESIUM	1CS	-0	-0	-0	-0		0	.0676	188
CESIUM (PURE CRYSTALINE)	1CS						0	.0676	189
CESIUM AZIDE	1CS	3N					-12	.0000	190
CESIUM CARBONATE	1C	3O	2CS				-821	.1521	191
CESIUM HYDRIDE	1CS	1H	-0	-0	-0		217	.1231	192
CESIUM PERCHLORATE	1CS	1CL	4O	-0	-0		-447	.1201	193
CESIUM TUNGSTEN FLUORIDE	6F	1CS	1W				-1160	.1770	194

CHLORINE TRIFLUORIDE	1CL	3F					-480	.0652	195
CHLORINE	2CL						-76	.0536	196
CHLORINE HEPTOXIDE	2CL	7O					300	.0000	197
CHLORINE MONOFLUORIDE	1CL	1F					-222	.0000	198
CHLORINE PENTAFLUORIDE (GAS)	1CL	5F					-427	.0000	199
CHLORINE PENTAFLUORIDE (CLF5)	1CL	5F					-464	.0642	200
CHLORINE TRIFLUORIDE	1CL	3F					-410	.0000	201
CHROMIUM	1CR	-0	-0	-0	-0		0	.2599	202
CIRCO LIGHT PROCESS OIL	32H	15C					-320	.0250	203
CIRCO LIGHT PROCESS OIL	32H	15C					-320	.0250	204
COPPER CHLORIDE	2CL	2CU					-328	.1270	205
COPPER OXIDE	1O	2CU					-278	.2160	206
COPPER CHROMITE	3O	1CU	1CR				0	.2150	207
COPPER HYDROXIDE	2H	2O	1CU				-1099	.1216	208
COPPER OXIDE (HYDRATED)	2H	2O	1CU				-1099	.1216	209
CUPRIC OXIDE	1CU	1O					-439		210
COPPER (PURE CRYSTALLINE)	1CU						0	.3223	211
CYANAMIDE	1C	2H	2N	-0	-0		219	.0000	212
CYANOGAUNYL AZIDE	2C	2H	6N				881	.0000	213
CYANOGEN (GASEOUS)	2C	2N					1414		214
CYCLOHEXYL AZIDE	6C	11H	3N				207	.0356	215
CYCLOPENTYL AZIDE	5C	9H	3N				385	.0353	216
CYCLOTETRAMETHYLENE TETRA HMX	8H	4C	8N	8O			61	.0686	217
DECADIBORANE	6H	2B					0	.0079	218
DECABORANE	10B	14H					-129	.0339	219
DEKADIAZENE	10B	22H	4N				-381	.0000	220
DIAMINO DIBORANE	2B	12H	2N				-745	.0000	221
DIAMINOGUANIDINE NITRATE	1C	8H	6N	3O			-239	.0000	222
DIAMINOGUANIDINIUM AZIDE(DAZAL	2C	8H	6N				741	.0513	223
DIAMMONIUM DECABORANE	10B	16H	2N				-450	.0000	224
DIAZIDOTRINITRAZAHEPTANEPATH	4C	8H	12N	6O			458	.0000	225
DIBORANE	2B	6H					354	.0000	226
DIBUTYL PHTHALATE	22H	16C	4O				-733	.0378	227
DIBUTYL PTHALATE	575C	790H	144O				-754	.0378	228
DIESEL OIL	22H	12C					-476	.0254	229
DIETHYL PHTHALATE	12C	14H	4O				-733		230
DIETHYL TRIAMINE	13H	4C	3N				-149	.0344	231
DIETHYLENE GLYCOL DINITRATE	4C	8H	2N	7O			-520	.0497	232
DIFLUOROAMINE	2F	1H	1N				-600	.0000	233
DIFLUOROMETHYLENEBISOXYFLUORID	1C	4F	2O				-1121	.0433	234
DIBORANE	2B	6H					179	.0158	235
DIETHYL PHTHALATE	14H	12C	4O				-832		236
DIETHYL PHTHALATE	14H	12C	4O				-832		237
DIBUTYL PHTHALATE	12C	22H	4O				-733		238
DICYANDIAMIDE	2C	4H	4N				85	.0505	239
DICYANO-2-BUTYNE-1,4	6C	4H	2N				841	.0415	240
DIHYDRONITRONITRIMINOPYRIDINE	5C	4H	4N	4O			143	.0650	241
DI-N-PROPYL ADIPATE	12C	22H	4O				-1164		242
DIMETHYL AMMON LITHIUM IODIDE	1LI	1I	4C	13H	1N		-477	.0000	243
DIMETHYL AMMON LITHIUM IODIDE	1LI	1I	6C	19H	1N		-473	.0000	244
DIMETHYL AMMON LITHIUM IODIDE	1LI	1I	10C	31H	1N		-463	.0000	245
DIMETHYLAMINE-BORANE ADDUCT	2C	10H	1B	1N			-516	.0000	246
DINITRO TOLUENE	6H	7C	2N	4O			-6200		247
DINITROPHENOXY ETHANOL	98H	104C	26N	75O			-271	.0565	248
DINITROPROPYL ACRYLATE	8H	6C	2N	6O			-514	.0471	249
DIOCTYL ADIPATE	42H	22C	4O				-733	.0332	250
DIOCTYL AZELATE	48H	25C	4O				-855		251
DIOCTYL AZELATE	48H	25C	4O				-855		252
DITRISDIFLUORCAMINOMETHYLUREA	3C	2H	12F	8N	1O		-203	.0679	253
DODECAHYDRODECABORATEDIAMMINE	10B	18H	2N				-564	.0361	254
DULCITOL	6C	14H	6O				-1740	.0530	255
DYNAMAR 732/746	970H	549C	11N	1430			-1420	.0376	256
DYNAMAR HX-73C	754H	445C	244O				-1200	.0420	257
DYNAMAR HX-743	942H	554C	80N	81O			-380	.0360	258
E107 (A MIXTURE)	441H	133C	52N	232O	6AL	49CL	-552	.0604	259
EPOXY 201	24H	16C	4O				-661	.0404	260

EPON 828	24H	21C	4O			0		261
ERYTHRITOL TETRANITRATE	4C	6H	4N	12O		-395	.0000	262
ESTANE	987H	536C	12N	140O		-910	.0379	263
ESTANE 6	55H	302C	1N	10O		-940	.0376	264
ETHANETHIOL	2C	6H	1S	-O	-O	-258	.0000	265
ETHANE(1,1-DINITRO)	2C	4H	2N	4O		-289	.0000	266
ETHANE(1,1,1-TRINITRO)	2C	3H	3N	6O		-166	.0552	267
ETHANE(1,2-BIS DIFLUOROAMINO)L	2C	4H	4F	2N		-356	.0000	268
ETHANE(1,2-BIS DIFLUOROAMINO)G	2C	4H	4F	2N		-310	.0000	269
ETHANE(1,2-DI TETRAZOLYL)	4C	6H	8N			639	.0000	270
ETHANOL	2C	6H	1O	-O	-O	-1440	.0000	271
ETHYL CENTRALITE	17C	20H	2N	1O		-127		272
ETHYLENE	2C	4H				289	.0205	273
ETHYLENE CARBONATE	3C	4H	3O			-1576	.0000	274
ETHYLENE DIHYDRAZINE	12H	2C	4N			346	.0396	275
ETHYLENE DINITRAMINE (EDNA)	2C	6H	4N	4O		-158	.0632	276
ETHYLENEBIS(AMINOGUANIDINEAZID	5C	16H	14N			496	.0000	277
FAPETRIN	6C	8H	6F	6N	1OO	-318	.0000	278
FAPETRIN	6C	8H	6F	6N	1OO	-268	.0000	279
FERRIC OXIDE (ANHYDROUS)*	3O	2Fe				-1230	.1818	280
FERRIC OXIDE HEMATITE	2FE	3O				-1235	.1848	281
FLOROX (CLF3O)	1O	3F	1CL			-371	.0666	282
FLUORINE	2F					-82	.0543	283
FLUORINE NITRATE	1F	1N	3O			31	.0000	284
FLUORINE (LIQUID)	2F					-76	.0543	285
FLUORO-2,2-DINITROETHANOL-2	2C	3H	1F	2N	5O	-741	.0000	286
FLUOROETHANE(1,1-DINITRO-1-)	2C	3H	1F	2N	4O	-488	.0000	287
FLUOROTRINITROMETHIDE	1C	1F	3N	6O		-221	.0573	288
FLUOROXYTRIFLUOROMETHANE	1C	4F	1O			-1769	.0000	289
FORMAMIDE	3H	1C	1N	1O		-1370	.0410	290
FREON 116 (ROGERS)	2C	6F				-2195		291
GASOLINE (LIQUID)	46H	21C				-794	.0257	292
GENPOL A-20	75H	555C	37OO			-1110		293
GILSINITE	866H	744C	6N	6S		-400	.0364	294
GLUTAMIC ACID	5C	9H	4O	1N		-1610	.0555	295
GUANIDINE	5H	1C	3N	-O	-O	-288	.0000	296
GUANADINE CARBONATE	3C	1OH	3O	6N		-1290		297
GUANIDINE NITRATE	6H	1C	4N	3O		-843	.0503	298
GUANIDINIUMNITRAMINOTETRAZLAT	2C	7H	9N	2O		141	.0000	299
GUANYLAZIDE NITRATE	1C	4H	6N	3O		26	.0000	300
H C BINDER (PAUL)	1O6H	71C	8N			-102		301
HEPTADYNE	8H	7C				-1127	.0293	302
HEXANE	14H	6C				-464	.0255	303
HEXACYANO-3-HEXENE	12C	6H	6N			862	.0444	304
HEXACYANO-3-HEXYNE	12C	4H	6N			1045	.0437	305
HEXACYANO-3,5-OCTADIYNE	14C	4H	6N			1146	.0466	306
HEXAKIS DIFLUOROAMINO DIPROPYL	8H	12F	6N	1O	6C	-315	.0596	307
HEXANE (2,2,5 TRIMETHYL)	2OH	9C				-537	.0246	308
HEXANITROETHANE (HNE)	2C	6N	12O			95	.0812	309
HMX	4C	8H	8N	8O		61	.0686	310
HTPB (SINCLAIR)	1O3H	73C	1O			13	.0332	311
HYCAR	139H	7OC	1O			-121	.0339	312
HYDRATED AMMONIUM PHOSPHATE	3N	18H	7O	1P		-3010		313
HYDROXYETHYL CELLULOSE	35H	22C	14O			-1200	.0464	314
HYDROXYL AMMONIUM NITRATE(NBS)	2N	3H	4O			-908		315
HYDROXYLAMMONIUMPERCHLORATE	1CL	4H	1N	5O		-497	.0767	316
HYDRAZINE NITRATE	5H	3N	3O			-531	.0595	317
HYDROXYL AMMONIUM NITRATE(NBS)	2N	3H	4O			-908		318
HYDRAZINE	4H	2N				376	.0364	319
HYDRAZINE AZIDE	5H	5N				727	.0470	320
HYDRAZINE CYANOFORMATE	4C	5H	5N			579	.0462	321
HYDRAZINE DIBUTANE	2B	1OH	2N			-500	.0339	322
HYDRAZINE HYDRATE (N2H4.H2O)	6H	2N	1O			-2900	.0378	323
HYDRAZINE NITROFORM	5H	1C	5N	6O		-95	.0676	324
HYDRAZINE(1,1-METHYLCYANOETHY	4C	9H	3N			339	.0353	325
HYDRAZINE(2)BORANE(8)COMPOUND	8B	28H	4N			-60	.0000	326

HYDRAZINE(3)BICRANE(10)COMPOUND	10B	24H	6N				-108	.0000	327
HYDRAZINE(4)BICRANE(10)COMPOUND	10B	26H	8N				-92	.0000	328
HYDRAZINE DIPERCHLORATE	6H	2N	8O	2CL			-309	.0797	329
HYDRAZINIUM DIPERCHLORATE	2CL	6H	2N	8O			-296	.0361	330
HYDRAZINIUM NITROFORMATE(HNF)	1C	5H	5N	6O			-94	.0671	331
HYDRAZINIUM PERCHLORATE	1CL	5H	2N	4O			-320	.0700	332
HYDRAZOBISISOBUTYRONITRILE	8C	14H	4N				172	.0000	333
HYDRAZOIC ACID (GASEOUS)	1H	3N					1635		334
HYDRAZOTETRAZOLE-5,5	2C	4H	10N				804	.0000	335
HYDROCARBON POLYMER	2H	1C					-339	.0332	336
HYDROGEN (GASEOUS)	2H						0		337
HYDROGEN AZIDE	1H	3N					1460	.0394	338
HYDROGEN AZIDE	1H	3N					1430	.0000	339
HYDROGEN CYANIDE (GASEOUS)	1H	1C	1N				932	.0248	340
HYDROGEN CYANIDE (LIQUID)	1H	1C	1N				1154	.0325	341
HYDROGEN FLUORIDE	1H	1F					-3581	.0357	342
HYDROGEN FREE RADICAL	1H						52090		343
HYDROGEN PEROXIDE (100 PC)	2H	2O					-1319	.0508	344
HYDROGEN PEROXIDE (50 PC)	850H	5720					-1927	.0430	345
HYDROGEN PEROXIDE (70 PC)	746H	5790					-1684	.0464	346
HYDROGEN PEROXIDE (90 PC)	642H	5760					-1439	.0501	347
HYDROGEN PEROXIDE (GASEOUS)	2H	2O					-958	.0000	348
HYDROGEN SULFIDE	2H	1S					-141	.0768	349
HYDROGEN (CRYOGENIC)	2H						-1068	.0026	350
HYDROXYETHYL METHACRYLATE	10H	6C	3O				-1200	.0420	351
HYDROXYL RADICAL	1H	1O	-0	-0	-0		591	.0000	352
HYDROXYLAMINE	3H	1N	1O				-793	.0000	353
HYDROXYETHYL CELLULOSE	35H	22C	14O				-1200	.0464	354
HYDROXYTERMINAT POLYBUTADIENE	103H	73C	1O				13	.0332	355
HYCAT (BENNETT)	36H	29C	2FE				40	.0441	356
HYCAT (BENNETT)	36H	29C	2FE				40	.0441	357
IDP (D. LEE)	38H	19C	2O				-908	.0312	358
IODIC ACID	1H	1I	3O	-0	-0		-324	.1671	359
IODINE	2I	-0	-0	-0	-0		0	.1760	360
IODINE PENTAFLUORIDE	5F	1I					-928	.1140	361
IODINE PENTOXIDE	5O	2I					-127	.1732	362
IODINE TRICHLORIDE	1I	3CL	-0	-0	-0		-90	.1125	363
IODOFORM (CHI3)	1H	1C	3I				-85	.1443	364
IRON OXIDE	3O	2FE					-1230	.1840	365
IRON OXIDE (YELLOW)	2H	4O	2FE				-1490	.1318	366
IRON	1FE						0	.2837	367
ISO OCTANE	18H	8C					-470		368
JP4 (LIQUID TURBOJET FUEL)	17H	9C					-281	.0254	369
JP5 (MONT STEVENS STANDARD)	19H	10C					-387	.0296	370
KRATON	4H	3C					-1073	.0340	371
KRATON STYRENE BUTADIENE	4H	3C					-1073	.0340	372
KRATON (CO-POLYMER)	6H	4C					-100	.0342	373
LAMINAC 4116	555H	558C	171O				-574		374
LEAD ACETYL SALICYLATE	14H	18C	6O	1PB			-857		375
LEAD OXIDE (MINIUM)	4O	3PB					-262	.3286	376
LEAD BETA RESORCYLATE	21H	7C	7O	1PB			0		377
LEAD OXIDE	1PB	1O					-235		378
LEAD IODATE	1PB	2I	6O				-267	.1913	379
LEAD SALICYLATE	10H	14C	6O	1PB			-84	.0337	380
LEAD 2-ETHYL HEXOATE	34H	16C	4O	1PB			0		381
LEAD 2-ETHYL HEXOATE	34H	16C	4O	1PB			0		382
LEAD AZIDE	6N	1PB					397	.0000	383
LEAD IODATE	1PB	2I	6O				-267	.1913	384
LEAD OXIDE (LITHARGE)	1O	1PB					-235	.3440	385
LEAD OXIDE (MASSICOT)	1O	1PB					-235	.2868	386
LEAD DIOXIDE	2O	1PB					-276	.3384	387
LEAD SALICYLATE	10H	14C	6O	1PB			-84	.0337	388
LEAD OXIDE (PLATTNERITE)	2O	1PB					-66	.3384	389
LITHIUM ALUMINUM HEXA HYDRIDE	1AL	6H	3LI				-1417	.0401	390
LITHIUM ALUMINUM PERCHLORATE	3LI	24O	1AL	6CL			-645	.0897	391
LITHIUM ALUMINUM TETRA HYDRIDE	1AL	4H	1LI				-690	.0331	392

LITHIUM AMIDE *	2H	1LI	1N			-1894	.0329	393
LITHIUM AZIDE	1LI	3N				57	.0000	394
LITHIUM BERYLLIUM HYDRIDE	1BE	4H	2LI			-2908	.0000	395
LITHIUM BOROHYDRIDE	1B	4H	1LI			-2131	.0246	396
LITHIUM CARBIDE	2LI	2C	-C	-0	-0	-375	.0596	397
LITHIUM CARBONATE	2LI	1C	30			-5900	.0762	398
LITHIUM DICYANAMIDE	2C	1LI	3N			-120	.0000	399
LITHIUM FLUORIDE	1LI	1F				-5620	.0939	400
LITHIUM HYDRIDE	1H	1LI				-2726	.0296	401
LITHIUM HYDROXIDE	1H	1LI	1O			-4868	.0917	402
LITHIUM NITRATE	1LI	1N	3O			-1670	.0859	403
LITHIUM NITRIDE	3LI	1N				-1355	.0498	404
LITHIUM PERCHLORATE (LICLO4)	1CL	1LI	4O			-854	.0877	405
LITHIUM PERIODATE	1LI	4O	1I			-490	.1520	406
LITHIUM (PURE CRYSTALINE)	1LI					0	.0193	407
LP-33	314C	655H	1070	121S		-696	.0458	408
LP-295	416C	846H	850	87S		-720	.0408	409
MAGNESIUM (PURE CRYSTALINE)	1MG					0	.0628	410
MAGNESIUM ALUMINUM HYDRIDE	2AL	8H	1MG			-365	.0378	411
MAGNESIUM BORIDE	2B	1MG				-478	.0970	412
MAGNESIUM CYANAMIDE	1MG	1C	2N	-0	-0	-937	.0000	413
MAGNESIUM FLUORIDE	2F	1MG				-2862	.1003	414
MAGNESIUM HYDRIDE	2H	1MG				-645	.0524	415
MAGNESIUM NITRATE	1MG	2N	6O	-0	-0	-1272	.0731	416
MAGNESIUM OXIDE	1O	1MG				-3610	.1300	417
MAGNESIUM PERCHLORATE	8O	1MG	2CL			-639	.0939	418
MAGNESIUM (NON-REACTIVE)	1O3					0	.0628	419
MAGNESIUM OXIDE	248MG	248O				-3567	.1292	420
MAPO (ARC)	18H	9C	1O	3N	1P	-266		421
N-BUTYL FERROCENE	18H	14C	1FE			10	.0430	422
MERCURIC FLUORIDE	2F	1HG				-398	.3216	423
MERCURIC OXIDE	1O	1HG				-100	.4023	424
MERCUROUS AZIDE	2HG	6N				292	.0000	425
MERCURY (LIQUID)	1HG					0	.4873	426
METHANE	1C	4H				-1271	.0153	427
METHANE*	4H	1C				-1118		428
METHANOL	4H	1C	1O			-1780	.0267	429
METHOXYAMINE	1C	5H	1N	1O		-276	.0000	430
METHYL ACRYLATE (LIQ.) -HC-	6H	4C	2O			-954	.0364	431
METHYL ALCOHOL	4H	1C	1O			-1781	.0265	432
METHYL AMMONIA	5H	1C	1N			-216	.0236	433
METHYLNITROACETATE	3C	5H	1N	4O		-922	.0000	434
MIXED HYDRAZINE FUEL 3	647H	93C	231N			297	.0323	435
MIXED OXIDES OF NITROGEN	63N	1010				43	.0520	436
MIXED HYDRAZINE FUEL 5	114H	12C	46N	6O		149	.0361	437
MIXED HYDRAZINE FUEL 3	647H	93C	231N			297	.0323	438
MON 25/75	175N	3250				69	.0498	439
MONOBASIC AMMONIUM PHOSPHATE	1N	6H	1P	4O		-3020	.0651	440
MONOBASIC CUPRIC SALICYLATE	14C	10H	7O	2CU		-700		441
MONOBASIC CUPRIC RESORCYLATE	14C	10H	9O	2CU		-2782		442
MONOBASIC LEAD RESORCYLATE	14C	10H	9O	2PB		-1900		443
MONOBASIC LEAD SALICYLAT	14C	10H	9O	2PB		-332		444
MONOMETHYL HYDRAZINE (MMH)	6H	1C	2N			276	.0316	445
N P AMINE	7H	6C	1N			-1287	.0329	446
NF4BF4	1B	1N	6F			-1640	.0853	447
NICKEL	1NI					0	.3215	448
NICKEL OXIDE	1O	1NI				-773		449
NICKEL CARBIDE	3NI	1C	-0	-0	-0	58	.2672	450
NICKEL CHLORIDE	2CL	1NI				-580	.1287	451
NITROGEN	2N					-104	.0292	452
NITROGEN TETROXIDE (N2O4) LIQ	2N	4O				0	.0517	453
NITROUS OXIDE	2N	1O	-C	-0	-0	447	.0714	454
NITROCELLULOSE (12.6PERCENT N)	755H	600C	245N	990O		-617	.0560	455
NITROGLYCERIN	3C	5H	3N	9O		-400	.0578	456
NITRATE	5H	3N	3O			-932		457
NITRIC ACID (GAS)	1H	1N	3O			-509	.0000	458

NITROAMINOGUANIDINE	1C	5H	5N	20		45	.0000	459
NITROETHANE	2C	5H	1N	20		-442	.0376	460
NITROGEN PENTOXIDE	2N	5O	-0	-0	-0	-93	.0593	461
NITROGEN TETROXIDE (GASEOUS)	2N	4O				24	.0000	462
NITROGEN TRIFLUORIDE	3F	1N				-416	.0000	463
NITROGEN TRIFLUORIDE	3F	1N				-460	.0502	464
NITROGUANYL AZIDE	1C	2H	6N	20		548	.0000	465
NITROMETHANE	1C	3H	1N	20		-443	.0000	466
NITRONITRAMINOPYRIDINIUMCLO4	5C	5H	1CL	4N	40	7	.0650	467
NITRONIUM ALUMINUM PERCHLORAT	1AL	6CL	3N	300		-160	.0000	468
NITRONIUM PERCHLORATE	1CL	1N	60			61	.0794	469
NITROPROPENE POLYMER	3C	5H	1N	20		-252	.0000	470
NITROSOAMINE(N,N-DIMETHYL)	2C	6H	2N	10		16	.0036	471
NITROSOL BINDER	143H	105C	40N	1640		-476	.0515	472
NITROSYL FLUORIDE	1F	1N	10			-324	.0000	473
NITROSYL PERCHLORATE	1CL	1N	50			-284	.0763	474
NITROSYL TETRAFLUOROCHLORATE	1CL	4F	1N	10		-489	.1029	475
NITROUREA	1C	3H	3N	30		-611	.0000	476
NITRYL FLUORIDE	1F	1N	20			-290	.0000	477
NITRYLTETRAFLUOROCHLORATE	1CL	4F	1N	20		-305	.0000	478
NITRIC ACID (LIQ)	1H	1N	30			-658	.0542	479
NITROGUANIDINE	1C	4H	4N	20		-209	.0000	480
N-AMYL ALCOHOL	5C	12H	1O			-922	+509	481
N-AMYL ALCOHOL	5C	12H	1O			-922	.0509	482
N-PHENYLMORPHOLINE	13H	10C	1N	10		-123	.0409	483
NORMAL HEPTANE	16H	7C				-449		484
N,N-DINITRO-N-BUTYLAMINE (DNBA	4C	9H	3N	40		-13	.0433	485
O2/H2 (O/F =10.6058)	289H	5940				0		486
O2/H2 (O/F =16.6058)	289H	5940				0		487
OCTANE	18H	8C				-470		488
OLEIC ACID (VEGETABLE OIL)-HC-	34H	18C	20			-723	.0323	489
OTTO FUEL 2	999H	430C	2N	5030		-696		490
OXAMID (B. LEE)	4H	2C	2N	20		-1376	.0602	491
OXYCHLORINE TRIFLUORIDE	1O	3F	1CL			-371	.0686	492
OXYCHLORINE TRIFLUORIDE	1O	3F	1CL			-360	.0669	493
OXYGEN (GAS)	2O					0		494
OXYGEN DIFLUORIDE	2F	1O				-155	.0549	495
OXYGEN DIFLUORIDE	2F	1O				-81	.0000	496
OXYGEN (LIQUID)	2O					-97	.0412	497
OZONE	3O					631	.0523	498
PENTABORANE (GASEOUS)	5B	9H				237	.0231	499
PENTABORANE (LIQUID)	5B	9H				122	.0000	500
PENTAERITHRITOL	5C	12H	4O			-1609	.0523	501
PENTAERYTHRITOL TETRANITRATE	5C	8H	4N	12O		-401	.0640	502
PENTAKIS(HYDRAZINE)DECABORANE	10B	34H	10N			40	.0000	503
PERCHLORIC ACID (ANHYDROUS)	1CL	1H	4O			-110	.0639	504
PERCHLORYL FLUORIDE (CLO3F)	1CL	1F	3O			-50	.0000	505
PERFLUORO METHACRYLATE	6H	8C	2O	8F		-1300	.0650	506
PERFLUOROFORMAMIDINE (PFF)	1C	4F	2N			-290	.0000	507
PERFLUOROGUANIDINE (PFG) (LIQ)	1C	5F	3N			127	.0000	508
PERFLUOROGUANIDINE (PFG) (GAS)	1C	5F	3N			162	.0000	509
PERFLUOROPIPERIDINE	5C	11F	1N			-1728	.0625	510
PERFLUOROPIPERIDINE	5C	11F	1N			-1703	.0000	511
PETRIN	9H	5C	3N	100		-513	.0557	512
PETRIN	9H	5C	3N	100		-513	.0557	513
PHENOXY	98H	104C	26N	750		271	.0565	514
PHENYL AZIDE	6C	5H	3N			694	.0343	515
PHOSPHORUS (RED)	1P					-136	.0794	516
PLASTISOL NITROCELLULOSE	755H	600C	245N	9900		-586	.0599	517
PLEXIGLASS	8H	5C	2O			-906	.0426	518
PNC	755H	600C	245N	9900		-586	.0599	519
POLYMETHYL VINYLTETRAZOLE	6H	4C	4N			470	.0462	520
POLYPROPYLEN GLYCOL	12H	6C	2O			-655		521
POLYETHYLENE	2C	4H				-453	.0325	522
POLYURETHANE BINDER	987H	536C	12N	1400		-910	.0379	523
POLYACRYLAMIDE	3C	5H	1N	1O		-1590	.0000	524

POLYACRYLONITRILE	3H	3C	1N				74	.0398	525
POLYAMINE COMPOSITE	30C	105H	25N				-316	.0342	526
POLYBUTADIENE (SEE BUTAREZ)	6H	4C					55	.0364	527
POLYBUTADIENE ACR A (THIOKOL)	999H	671C	19N	160			-160	.0330	528
POLYTETRAFLUOROETHYLENE	2C	4F					-1952	.0834	529
POLYETHYLENEHYDRAZINE (PEH)	2C	6H	2N				4	.0000	530
POLYPROPYLEN GLYCOL	12H	6C	2O				-855		531
POLYBUTADIENE ACRYLIC ACID	104H	70C	4O				-84	.0337	532
POTASSIUM PERCHLORATE (KCLO4)	1CL	1K	4O				-742	.0910	533
POTASSIUM PERCHLORATE (KCLO4)	1CL	1K	4O				-742	.0910	534
POTASSIUM IODATE	3O	1K	1I				-568	.1405	535
POTASSIUM SULFATE	4O	1S	2K				-1966	.0962	536
POTASSIUM	1K						0	.0500	537
POTASSIUM AMALGAM	1K	1Hg	-0	-0	-0		-48	.0000	538
POTASSIUM AZIDE	1K	3N					-5	.0736	539
POTASSIUM CARBONATE	1C	3O	2K				-1495	.0877	540
POTASSIUM CHLORIDE	1CL	1K					-1397	.0717	541
POTASSIUM FERRICYNANIDE	3K	1Fe	6C	6N	-0		-126	.0684	542
POTASSIUM HYDRIDE	1K	1H	-0	-0	-0		-339	.0516	543
POTASSIUM NITRATE	1N	3O	1K				-1167	.0767	544
POTASSIUM IODATE (KIO3)	1K	1I	3O				-568	.1405	545
POTASSIUM PEROXIDE	2K	2O	-0	-0	-0		-1071	.0000	546
POTASSIUM SULFATE	4O	1S	2K				-1966	.0962	547
POTASSIUM SULFIDE	2K	1S	-0	-0	-0		-707	.0652	548
PROPANE	8H	3C					-591		549
PROPYL NITRATE	7C	3C	1N	3O			-514	4.298	550
PROPANE(1,1-DINITRO) (LIQUID)	3C	6H	2N	4O			-297	.0455	551
PROPANE(1,1-DINITRO) (GASEOUS)	3C	6H	2N	4O			-166	.0000	552
PROPANE(1,1,1-TRINITRO)	3C	5H	3N	6O			-157	.0000	553
PROPANE(1,1,1,3-TETRANITRO)	3C	4H	4N	8O			-172	.0000	554
PROPANE(1,2-BIS DIFLUOROAMINO)	3C	6H	4F	2N			-349	.0000	555
PROPANE(1,2-BIS DIFLUOROAMINO)	3C	6H	4F	2N			-294	.0000	556
PROPANE(1,3-DINITRO)	3C	6H	2N	4O			-399	.0469	557
PROPANE(2-NITRO)	3C	7H	1N	2O			-491	.0355	558
PROPANE(2,2-DINITRO)	3C	6H	2N	4O			-338	.0469	559
PROPYLENE POLY GLYCOL DIACRYL	102H	54C	19O				-1000	.0379	560
PROPANE(1-NITRO)	3C	7H	1N	2O			-448	.0353	561
P-QUINONEDIOXIME	434C	434H	145O	145N			-700	.0505	562
RDX(HEXAHYDROTRINITROTRIAZINE)	3C	6H	6N	6O			66	.0656	563
RED FUMING NITRIC ACID (14NO2)	151H	165N	471O				-654	.0567	564
RED FUMING NITRIC ACID (CORO2)	85H	114N	314O				-544	.0567	565
RED FUMING NITRIC ACID (14NO2)	151H	165N	471O				-654	.0567	566
RP-1	2H	1C					-1340	.0269	567
RESORCINOL	6H	6C	2O				-784	.0463	568
RUBIDIUM	1RB	-0	-0	-0	-0		0	.0553	569
SEA WATER	998H	499O	1NA	1MG	1CL		-3792	.0361	570
SILICON DIOXIDE (PURE MOJAVE)	2O	1Si					-3418	.0759	571
SILICON TETRACHLORIDE	1SI	4CL	-0	-0	-0		-901	.0535	572
SILICON (PURE CRYSTALINE)	1SI						0	.0874	573
SILVER IODATE	3O	1I	1AG				-149	.2010	574
SILVER IODATE	3O	1I	1AG				-149	.2010	575
SILVER METAL	1AG						0	.3791	576
SILVER NITRATE	1AG	1N	3O	-0	-0		-172	.1571	577
"S-06"	308C	864H	295O				-1145	.0523	578
"S-02"	141C	704H	352O	141N			-1397	.0542	579
SODIUM ALUMINUM AMIDE	1AL	8H	4N	1NA			-1520	.0000	580
SODIUM AZIDE	3N	1NA					60	.0668	581
SODIUM BARBITURATE	3H	4C	2N	3O	1NA		-1393	.0793	582
SODIUM BROMHYDRIDE	1B	4H	1NA				-1206	.0390	583
SODIUM CARBONATE	1C	3O	2NA				-821	.0914	584
SODIUM CHLORATE	1NA	1CL	3O	-0	-0		-805	.0899	585
SODIUM CHLORIDE	1NA	1CL					-1672	.0762	586
SODIUM FLUORIDE	1F	1NA					-3245	.1008	587
SODIUM HYDRIDE	1NA	1H	-0	-0	-0		-571	.0504	588
SODIUM IODATE (AW - DHSKIOS)	NA1	11	03				-535	.1544	589
SODIUM PERCHLORATE	4O	1NA	1CL				-750		590

SODIUM PEROXIDE	2NA	2O	-O	-O	-O	-1546	.1011	591
SODIUM POTASSIUM LIQ ALLOY	3K	1NA	-O	-O	-O	-43	.0000	592
SODIUM THIOCYANATE	1NA	1C	1N	1S	-O	-515	.0000	593
SODIUM (PURE CRYSTALINE)	1NA					0	.0350	594
SPAN 85	30H	15C	1O			-685	.0540	595
STYRENE	8H	8C				80	.0358	596
SUCCINIC ACID	4C	6H	4O			-1900	.0567	597
SULFUR	1S					0	.0747	598
SULFUR DIOXIDE	1S	2O	-O	-O	-O	-1108	.1057	599
SULFUR TRIOXIDE	1S	3O	-O	-O	-O	-1307	.0993	600
SULFUR (MONOCLINIC)	1S	-O	-O	-O	-O	2	.0706	601
SULFURIC ACID	2H	1S	4O	-O	-O	-1977	.0662	602
SULPHUR	1S					0	.0730	603
TETRAHYDRONAPTHALENE	12H	10C				-13	.0354	604
TETRACYANOCYCLOPROPANE1,1,2,2	7C	2H	4N			1007	.0495	605
TETRACYANOETHYLENE	6C	4N				1174	.0469	606
TETRAETHYLPENTAMINEPERCHLORATE	28H	8C	5N	2O	5CL	-545	.0470	607
TETRAETHYL LEAD	20H	8C	1PB			161	.0599	608
TETRAFLUOROHYDRAZINE (N2F4)	4F	2N				-19	.0000	609
TETRAKIS AMLY ACRYLATE (TAA)	9C	10H	8F	4N	2O	-396	.0530	610
TETRAKIS DIFLUORAMINOMETHANE	1C	8F	4N			18	.0631	611
TETRAKIS DIFLUORAMINOMETHANE	1C	8F	4N			12	.0000	612
TETRAKIS(DIFLUORAMINO) (THF)	4C	4H	8F	4N	1O	-266	.0579	613
TETRAKIS(HYDRAZINE)DECABORANE	10B	30H	8N			-10	.0000	614
TETRAMETHYL LEAD	12H	4C	1PB			202	.0721	615
TETRAMETHYLAMINOTRIBOROHYDRIDE	4C	20H	3B	1N		-293	.0000	616
TETRAMETHYLTRICYCLODECYLENEDIA	14C	26H	2N			-145	.0352	617
TETRANITRO DIFLUOROETHANE	2C	2F	4N	8O		-368	.0000	618
TETRANITRO METHANE	1C	4N	8O			45	.0593	619
TETRANITROETHYLENEDIAMINE	2C	4H	6N	8O		198	.0632	620
TETRANITROMETHANE	1C	4N	8O			45	.0592	621
TETRAZOLE	1C	2H	4N			809	.0000	622
TETRAZOLE(2-METHYL-5-AMINO)	2C	5H	5N			502	.0000	623
TETRAZOLE(5-AMINO)	1C	3H	5N			585	.0596	624
TETRAZOLE(5-CYANO)	2C	1H	5N			1010	.0000	625
TETRAZOLE(5-HYDROXY)	1C	2H	4N	1O		-17	.0000	626
TETRAZOLE(5,5-HYDRAZO)	2C	4H	10N			800	.0000	627
THORIUM	1TH	-O	-O	-O	-O	0	.4043	628
TIN (GREY)	1SN					0	.2076	629
TITANIUM DIOXIDE	1TI	2O				-2551		630
TITANIUM	1TI	-O	-O	-O	-O	0	.1624	631
TITANIUM BORIDE	2B	1TI				-1000	.1626	632
TITANIUM DIBORIDE	2B	1TI				-973	.1625	633
TMETN	5C	9H	3N	9O		-415	.0537	634
TMETN	5C	9H	3N	9O		-415	.0537	635
TOLUENE DIISOCYANATE	6H	9C	2N	2O		-855		636
TOLUENE DIAMINE	13H	7C	2N			-16	.0449	637
TOLUENE DIISOCYANATE	6H	9C	2N	2O		-855		638
TRIACETIN	14H	9C	6O			-1334	.0419	639
TRIACETIN	14H	9C	6O			-1334	.0419	640
TRIAMINOGUANIDINE	9H	1C	6N			553	.0564	641
TRIAMINOGUANIDINE NITRATE TAGN	1C	9H	7N	3O		-69	.0555	642
TRIAMINOGUANIDINE (TAG)	1C	8H	6N			553	.0563	643
TRIAMINOGUANIDINECYANOFORMATE	5C	9H	9N			603	.0516	644
TRIAMINOGUANIDINEDICYANAMIDE	2C	9H	9N			591	.0505	645
TRIAMINOGUANIDINIUM AZIDE (TAZ)	1C	9H	9N			718	.0520	646
TRIAMINOGUANIDINIUM TRIBOROHYD	1C	17H	3B	6N		329	.0000	647
TRIAMINOGUANIDINIUM NONABOROHYD	1C	23H	9B	6N		131	.0000	648
TRIAMINOGUANIDINIUM DECABOROHYD	1C	26H	10B	8N		120	.0000	649
TRIAMINOMELAMINE	9H	3C	9N			550	.0589	650
TRIAZOETHANOL*2	2C	5H	3N	1O		258	.0415	651
TRICALCIUM PHOSPHATE	8O	3CA	2P			-3156		652
TRICYANO*3*BUTENE*1,1,1	7C	3N	3N			846	.0433	653
TRICYANO*3*BUTYNE*1,1,1	7C	3H	3N			1128	.0433	654
TRICYANOETHANE*1,1,1	5C	3H	3N			807	.0430	655
TRICYANOETHYLENE	5C	1H	3N			1019	.0433	656

TRICYANOTRIAZINE'S	6C	6N				1006	.0502	657
TRICYCLODECYLINEDIAMINE	10C	18H	2N			-173	.0390	658
TRIETHYLAMINE	15H	6C	1N			-667		659
TRIETHYLENEGLYCOLDINITRATE	12H	6C	2N	8O		-645	.0457	660
TRIFLUORCAPINE OXIDE	3F	1N	1O			-413	.0000	661
TRIFLUORCMETHYL HYPOFLUORITE	1C	4F	1O			-1733	.0000	662
TRIMETHYLAMINEBORANE	3C	12H	1B	1N		-468	.0296	663
TRIMETHYLENE ALANE	3C	12H	1AL	1N		-285	.0000	664
TRIMETHYLOLETHANETRINITRATE	9H	5C	3N	9O		-397	.0557	665
TRANS-DIMETHYL-AZOTETRAZOLE	4C	6H	10N			975	.0000	666
TRINITRO'3'HYDROXYBUTANOL	4C	7H	3N	8O		-373	.0000	667
TRINITROETHYL NITRATE (TNEN)	2C	2H	4N	9O		-132	.0596	668
TRINITROHYDROXYBUTYRICACID	4C	5H	3N	9O		-672	.0000	669
TRINITROMETHANE (NITROFORM)	1C	1H	4N	6O		-61	.0576	670
TRISDIFLUOROAMINOFLUOROMETHAN	1C	2F	3N			-281	.0563	671
TRIS(AMMONIA)DECABORANE(14)	10B	26H	3N			-530	.0000	672
TRIS(DIFLUOROAMINO)BUTANE	4C	7H	6F	3N		-273	.0433	673
TRIS(DIFLUOROAMINO)FLUOROMETHA	1C	2F	3N			-245	.0000	674
TRIS(DIFLUOROAMINO)PROPANE	14H	9C	6N	3O	12F	-411	.0556	675
TUNGSTEN (PURE CRYSTALINE)	1W					0	.6969	676
TUNGSTEN OXIDE	1W	3O				-831		677
TURPENTINE	16H	10C				-119	.0296	678
UNSYM-DIFLUORUREA (UDFU)	1C	2H	2F	2N	1O	-705	.0000	679
UNSYM-DIMETHYLHYDRAZINE (UDMH)	2C	8H	2N			198	.0263	680
URANIUM	1U	-0	-0	-0	-0	0	.6751	681
URANIUM ALUMINUM (ALLOY)	2AL	1U				-76	.2939	682
URANIUM ALUMINUM (ALLOY)	3AL	1U				-105	.2461	683
URANIUM ALUMINUM (ALLOY)	4AL	1U				-129	.2163	684
UREA OXALATE	4C	10H	6O	4N		-1740		685
UREA	1C	4H	1O	2N		-1326	.0462	686
VANADIUM OXIDE	5O	2V				-2488		687
VITONA	10C	7H	13F			-1801	.0050	688
VITEL 207 (LEE)	35H	28C	10O			-729	.2240	689
VITON-TEFLON (1/3 MIXTURE)	22H	10OC	17OF			-1895	.0730	690
WATER	2H	1O				-3792	.0361	691
YELLOW IRON OXIDE	2H	4O	2FE			0		692
ZIRCONIUM	1ZR					0	.2311	693
ZIRCONIUM BORIDE	2B	1ZR				-654	.2199	694
ZIRCONIUM CARBIDE	1ZR	1C	-0	-0	-0	-436	.2450	695
ZIRCONIUM DIBORIDE	2B	1ZR				-680	.2200	696
ZIRCONIUM HYDRIDE	2H	1ZR				-444	.2024	697
						0		698
SUPPLEMENTARY LIST. CAUTION.						0		699
						0		700
'S-02'	141C	704H	3520	141N		-2397	.0542	701
'S-06'	360C	884H	2950			-1145	.0523	702
ALUMINUM OXIDE	2AL	3O				-4000	.3670	703
AMMONIUM SULFATE	2N	8H	1S	4O		-2140	.0639	704
AMMONIUM PERCHLORATE	340H	340O	85N	85CL		-590	.0704	705
AMMONIATED COPPER NITRATE	1CU	4N	6O	6H	-0	630	.000	706
AMMONIATED COPPER NITRATE	1CU	6N	6O	12H	-0	769	.000	707
AMMONIATED COPPER NITRATE	1CU	8N	6O	18H	-0	822	.000	708
AMMONIATED ALUMINUM IODIDE	1AL	3I	1N	3H	-0	262	.000	709
AMMONIATED ALUMINUM IODIDE	1AL	3I	3N	9H	-0	454	.000	710
AMMONIATED ALUMINUM IODIDE	1AL	3I	5N	15H	-0	592	.000	711
AMMONIATED ALUMINUM IODIDE	1AL	3I	6N	18H	-0	622	.000	712
AMMONIATED ALUMINUM IODIDE	1AL	3I	7N	21H	-0	645	.000	713
AMMONIATED ALUMINUM IODIDE	1AL	3I	9N	27H	-0	676	.000	714
AMMONIATED ALUMINUM IODIDE	1AL	3I	13N	39H	-0	722	.000	715
AMMONIATED ALUMINUM IODIDE	1AL	3I	20N	60H	-0	782	.000	716
AMMONIATED BERYLLIUM IODIDE	1BE	2I	4N	12H	-0	642	.000	717
AMMONIATED BERYLLIUM IODIDE	1BE	2I	6N	18H	-0	692	.000	718
AMMONIATED BERYLLIUM IODIDE	1BE	2I	13N	39H	-0	792	.000	719
AMMONIATED MAGNESIUM IODIDE	1MG	2I	6N	6H	-0	500	.000	720
AMMONIATED CALCIUM IODIDE	1CA	2I	1N	3H	-0	507	.000	721
AMMONIATED CALCIUM IODIDE	1CA	2I	2N	6H	-0	570	.000	722

AMMONIATED CALCIUM IODIDE	1CA	2I	6N	18H	-0	727	.000	723
AMMONIATED CALCIUM IODIDE	1CA	2I	6N	24H	-0	735	.000	724
AMMONIATED LITHIUM IODIDE	1LI	1I	1N	3H	-0	609	.000	725
AMMONIATED LITHIUM IODIDE	1LI	1I	2N	6H	-0	691	.000	726
AMMONIATED LITHIUM IODIDE	1LI	1I	3N	9H	-0	751	.000	727
AMMONIATED LITHIUM IODIDE	1LI	1I	4N	12H	-0	799	.000	728
AMMONIATED LITHIUM IODIDE	1LI	1I	5N	15H	-0	825	.000	729
AMMONIATED LITHIUM IODIDE	2LI	2I	11N	33H	-0	417	.000	730
AMMONIATED LITHIUM IODIDE	1LI	1I	7N	21H	-0	857	.000	731
AMMONIUM CYANIDE	2N	4H	1C	-0	-0	0	.000	732
ARGON	1AR	-0	-0	-0	-0	0	.000	733
BARIUM NITRATE	1BA	2N	6O	-0	-0	907	.117	734
BARIUM PEROXIDE	1BA	2O	-0	-0	-0	889	.179	735
BERYLLIUM NITRIDE	3BE	2N	-0	-0	-0	2404	.000	736
CALCIUM CARBIDE	1CA	2C	-0	-0	-0	234	.000	737
CALCIUM NITRATE	1CA	2N	6O	-0	-0	1305	.000	738
CALCIUM PEROXIDE	1CA	2O	-0	-0	-0	2105	.000	739
CARBON (AMORPHOUS)	1C					917	.0637	740
CARBON MONOXIDE	1C	1O	-0	-0	-0	943	.045	741
DECAHYDRONAPTHALENE	10H	10C				-421	.0319	742
DIBUTYL TIN MALEATE	20H	12C	4O	1SN		-931	.0528	743
DIMETHYL AMMON LITHIUM IODIDE	1LI	1I	4C	13H	1N	477	.000	744
DIMETHYL AMMON LITHIUM IODIDE	1LI	1I	6C	19H	1N	473	.000	745
DIMETHYL AMMON LITHIUM IODIDE	1LI	1I	10C	31H	1N	463	.000	746
ERL-0510	19H	15C	1N	4O		-188	.0444	747
ETHANETHIOL	2C	6H	1S	-0	-0	250	.000	748
HC 434 VICTOR	75H	50C	1O			134		749
HYDROGEN CYANIDE	1H	1C	1N	-0	-0	1154	.032	750
HYDROGEN CYANIDE	1H	1C	1N	-0	-0	952	.024	751
LEAD NITRATE (LEE)	2N	6O	1PB			-324	.1637	752
LITHIUM HYDRIDE	1LI	1H	-0	-0	-0	2719	.023	753
LP-205	416C	646H	85O	87S		-720	.0456	754
LP-35	214C	83H	107O	12IS		-696	.0453	755
MAGNESIUM OXIDE	240MG	480				-3567	.1242	756
METHANE	1C	4H	-0	-0	-0	1115	.000	757
MONOBASIC LEAD RESORCYLATE	14C	10H	9O	2PB		-1900		758
NITROUS OXIDE	2N	1O	-0	-0	-0	443	.071	759
O2/H2 (O/F =1.00(5c)	00H	5240				0		760
OZONE	3O	-0	-0	-0	-0	702	.077	761
P-QUINONEDIOXIME	4540	404H	1450	145N		-700	.0505	762
POLYMERIZED FORMALDEHYDE	2H	1C	1O			-1343	.0509	763
USE SERIAL 535 FOR KCLO4******						0		764
POTASSIUM NITRATE	1K	1N	3O	-0	-0	1165	.076	765
POTASSIUM AMALGAM	1K	1HG	-0	-0	-0	48	.000	766
SILICONE	6H	2C	1O	1SI		-1820	.0361	767
SODIUM NITRATE	1N	3O	1NA			-1312	.0616	768
SODIUM BROMHYDRIDE	1NA	1B	4H	-0	-0	1155	.038	769
SODIUM HYDRIDE	1NA	1H	-0	-0	-0	571	.050	770
SODIUM NITRATE	1NA	1N	3O	-0	-0	1312	.061	771
TEFLON	1C	2F				-1930	.0794	772
TITANIUM	1TI	-0	-0	-0	-0	0	.162	773
URANIUM	1U	-0	-0	-0	-0	0	.314	774
VITON A	236H	274C	342F			-1890	.0656	775
VITEL (DIEBOLD)	35H	28C	10O			-1720	.0439	776
JP5 (OLD, SEE MONT STEVENS)	16H	9C				-278	.0296	777
INFNA 62.8AC 14NO2 2.9H2O .7HF	4F	166H	185N	5360		-541	.0507	778
SUCROSE (TABLE SUGAR)	22H	12C	11O			-1550	.0574	779
POLYMERIZED FORMALDEHYDE	2H	1C	1O			-1343	.0509	780
ALUMINUM OXIDE	2AL	3O				-4000	.0670	781
ERL-0510	19H	15C	1N	4O		-188	.0444	782
HC 434 VICTOR	75H	50C	1O			134		783
LEAD (PURE CRYSTALINE)	1PB					0	.4096	784
LEAD NITRATE (LEE)	2N	6O	1PB			-324	.1637	785
VITON A	236H	274C	342F			-1890	.0656	786
CARBON BLACK	1C					0	.0637	787
DIBUTYL TIN MALEATE	20H	12C	4O	1SN		-931	.0528	788

(LEN LEE ORDERED THE CARD THAT USED TO BE HERE DESTROYED.)							0		789
HTPE (SIMCLAIR)	10 3H	73C	1O				13	.0332	790
POLYSULFIDE LPC	12 9C	242H	4CO	4CS			-569	.0455	791
CARBON SUBNITRIDE	4C	2N					1970	.0390	792
CALCIUM FORMATE	2H	2C	4O	1CA			-2469	.0726	793
HELIUM	1HE						0	.0012	794
POLYSULFIDE LPC	12 9C	242H	4CO	4CS			569	.0456	795
TETRAFORMALTRISAZINE	4C	12H	6N				583	.0472	796
AMMONIUM BICARBONATE (NH4HCO3)	1H	2N	4O	1CO			-271	.0939	797
CTFE(ARC ICKPC/MIAA PAPER)	579C	964H	22O	5N	1P		-342	.0324	798
LAURYL METHACRYLATE	32H	17C	2O				-709	.0314	799
OXALIC ACID	2C	4O	2H				-2195	.0686	800
OXALIC ACID DIHYDRATE	2C	6O	6H				-2704	.0597	801
ANTHRACENE	10H	14C					152	.0451	802
DECACYLENE	16H	30C					117	.0596	803
SILVER IODIDE	1AG	1I					-64	.2049	804
SILVER OXIDE	2AG	1O					-32	.2581	805
NITROGEN (GASEOUS)	2N						0		806
SYFO	14H	11C	6N	10O	1OF		-441	.0542	807
PCDE	2H	3C	2N	1O	2F		-198	.0549	808
FEFO	6H	5C	4N	1OO	2F		-557	.0576	809
N-BUTANE (GAS)	10H	4C					-517		810
SODIUM HYDROXIDE	1NA	1O	1H				-2548	.0709	811
NAPTHALENE	10C	8H					164	.0413	812
CARBON TETRAFLOURIDE (GAS)	1C	4F					-2505		813
BILL BURDETTE- PAT HALL FUELS							0		814
ISOBUTYLBENZENE (USE 1054)	10C	14H					-12	.0313	815
DECAHYDRONAPTHALENE	18H	10C					-421	.0319	816
TETRAHYDRONAPTHALENE	12H	10C					-17	.0354	817
METHYL NAPTHALENE (1-)	10H	11C					9	.0370	818
THIOPHEN	2OH	12C					-198	.0334	819
SHELLDYNE H	124H	140C					107	.0390	820
N-BUTYL BENZENE (PENSON)	10C	14H					-119	.0313	821
N-BUTYL BENZENE (LANGE)	10C	14H					-139	.0313	822
AMSCO 140H SOLVENT	6C	12H					-437	.0292	823
SHELLDYNE-BUTYLBENZENE (1-1)	991H	749C					64	.0362	824
TETRALIN-DECALIN (70-30)	999H	726C					-135	.0342	825
METHYLIN-TETRALIN (70-30)	106H	107C					2	.0305	826
DECALIN-TETRALIN (80-20)	999H	576C					-239		827
THE FOLLOWING DATA WAS KINDLY PROVIDED BY ED LAFOUTY OF NOS							0		828
IT IS PREPARED FROM REPEATED HEAT OF COMBUSTION DATA							0		829
							0		830
1,1,1-TRINITRO-2-HYDROXYBUTYRIC	04C	05H	09O	03N			-684		831
C ACID							0		832
1,3,5-NITROXY-2-NITROAMINO-DIAZ	04C	07H	09O	05N			-156		833
ZACYCLOHEXENE							0		834
1,1,1-TRINITRO-2-HYDROXYBUTANOL	04C	07H	08O	03N			-373		835
L							0		836
1,2-BIS(DIFLUORAMINO)-2-METHYL	04C	06H	02N	04F			-389		837
PROPANE							0		838
1-DIFLUORAMINO-2,4,6-TRINITROB	06C	02H	08O	04N	2OF		19		839
BENZENE							0		840
1,1-DIMETHYL HYDRAZINE NITRATE	02C	09H	03O	3N			-470		841
1,2-BIS(DIFLUORAMINO)BUTANE	04C	08H	02N	4F			-341		842
1,1,1-TRINTRO-4,4-BIS(DIFLUORO	05C	07H	06O	05N	4F		-197		843
AMION)PENTANE							0		844
2-METHYL-5-VINYLTETRAZOLE ACRY	363C	541H	81O	54IN			357		845
LIC ACID COPOLYMER(15:1)							0		846
2-METHYL-5-METHOXYETHYLETETRAZ	358C	745H	057O	2O2N			-166		847
OLE							0		848
2-NITRO-5-HYDROXY-1,2,4-TRIAZO	02C	02H	03O	04N			-238		849
LE							0		850
2,3-DIFLUOROAMINO-2-METHYLBUTA	05C	10H	02N	04F			-336		851
NE							0		852
(2,2,2-FLUORODINITROETHYL)ACRY	05C	05H	08O	02N	04F		-669		853
LATE							0		854

2,4-DINITROPHENOXY ETHANOL	C08C	08H	C060	002N		-419		655
3-DIFLUORAMINO-2,4,6-TRINITRO	C7C	C04H	CC60	C04N	C02F	-7		656
TOLUENE						0		657
XYLIDINE	C03C	011H	001N			-144		658
2-FLUORO-2,3-DINITROETHANOL	C02C	003H	C050	002N	C01F	-741		659
2-HYDROXY-4(2-HYDROXY-3-METHAC	C20C	020H	0060			-722		660
RYLYLOXY)-PROPOXYBENZOPHENONE						0		661
2,2',4,4',6,6'-HEXANITROAZOBEN	C12C	004H	0120	006N		135		662
ZENE						0		663
2-METHYL-5-VINYLTETRAZOLE	C04C	006H	C04N			566		664
2-METHYL-5-VINYLTETRAZOLE/HYDR	377C	5C6H	0350	311N		252		665
OXY-ETHYL-METHACRYLATE COPOLYM						0		666
ER(1C:1)						0		667
2,2-DINITRO-2-CHLOROETHANOL	C02C	C03H	0050	002N	C01CL	-348		668
2,3-BUTANEDIOL	C04C	010H	C020			-1445		669
5-HYDROXYETHYL-1-1-METHYLTETRA	C04C	008H	0010	004N		7		670
ZOLE						0		671
5-NITROBARBITARIC ACID	175C	390H	3200	169N		-1625		672
5-AMINOTETRAZOLE NITRATE	C01C	C04H	0030	006N		130		673
5-AMINOTETRAZOLE PERCHLORATE	C01C	004H	0040	005N	001CL	204		674
A COMMERCIAL FLUOROCARBON	249C	139H	CC20	3C0F		-1858		675
A PARAFFINIC OIL	077C	124H				-367		676
A PHOSPHITED POLYALKYL POLYPHE	C67C	109H	0040	000N		-368		677
NOL						0		678
A NAPHTHENIC TYPE OIL	073C	117H				-167		679
A SUBSTITUTED ACRYLONITRILE	018C	015H	C020	001N		-103		680
ACETYLTRIBUTYL CITRATE	C20C	034H	0060			-1097		681
ACRYLAMIDE	003C	005H	0010	001N		-753		682
ACRYLONITRILE	575C	609H	0080	169N		334		683
ADAMANTANE	010C	016H				-340		684
BISTETRAZOLE	C02C	002H	C08N			1093	.0576	685
BIS-2,2-METHOXYETHOXY ETHYL ET	010C	022H	0050			-966		686
HER						0		687
BIS(2-FLUORO-2,2-DINITROETHYL)	C04C	005H	0080	005N	C02F	-439		688
AMINE						0		689
BIS(2-FLUORO-2,2-DINITROETHYL)	C04C	004H	0100	006N	C02F	-361		690
NITRAMINE						0		691
BIS(2-FLUORO-2,2-DINITROETHYL)	C04C	004H	0090	006N	C02F	-321		692
NITROSAMINE						0		693
BIS(2,2,2-TRINITROETHYL)SEBACAT	014C	020H	0160	006N		-409		694
BIS(2-FLUORO-2,2-DINITROETHYL)	C06C	006H	0100	006N	C02F	-645		695
OXAMIDE						0		696
BIS(2-FLUORO-2,2-DINITROETHYL)	C06C	004H	0120	004N	C02F	-798		697
OXALATE						0		698
CASTOR DIOL(HYDROXY NO.273-295	C59C	111H	11CH			-671		699
CARBOXYTERMINATED POLYBUTADIENE	073C	135H	0010			117		900
						0		901
CARBOXY TERMINATED POLYISOBUTY	070C	135H	0010			-450		902
LENE						0		903
CARBOXY TERMINATED POLYBUTADIE	072C	138H	0010			160		904
NE						0		905
CARBOXY TERMINATED POLYBUTADIE	091C	928H	0010	005N		-56		906
NE NITRILE						0		907
CARBOXY TERMINATED POLYBUTADIE	068C	962H	053N			-143		908
NE NITRILE						0		909
CARBOXY TERMINATED POLYBUTADIE	069C	103H	0190	030N		-29		910
NE NITRILE						0		911
CARBOXY TERMINATED POLYBUTADIE	068C	999H	0130	034N		33		912
NE NITRILE						0		913
CARNAUBA WAX	067C	127H	0040			-460		914
CANDELLIA WAX	069C	122H	0030			-142		915
CUMENE HYDROPEROXIDE	062C	830H	0940			-471		916
DELRIN	334C	664H	0330			-1373		917
DIHYDROXYGLYOXIME	002C	004H	C040	002N		-1080		918
DIETHYLENEGLYCOL DINITRATE	C04C	008H	0070	002N		-500		919
DIETHYLENE GLYCOL MONOBUTYLETH	010C	020H	0040			-1055		920

ERACETATE					0	921
DIETHYLENE GLYCOL DIMETHYL ETH	C06C	014H	0030		-1014	922
ER					0	923
DIPROPYLENE GLYCOL ESTER OF SE	U63C	064H	0670		-293	924
BACIC AND MALIC ACIDS					0	925
DIMETHYLACETAMIDE	004C	009H	0010	001N	-819	926
DIOXANE	442C,	074H	1037C		-935	927
DIETHYLOXALATE	006C	010H	0040		-1324	928
DIBASIC LEAD PHTHALATE	008C	004H	0000	003PB	-292	929
DIETHYL PHTHALATE	012C	014H	0040		-810	930
DI-ISOBUTYL ADIPATE	017C	032H	0040		-925	931
ETHANOLAMINE	002C	007H	0010	001N	-1986	932
ETHYLENEDIAMINE DIPERCHLORATE	002C	010H	0080	002N 002CL	-439	933
ETHYL ACRYLATE	005C	008H	0020		-877	934
ETHYLACRYLATE ACRYLIC ACID	495C	706H	2040		-1067	935
ETHYL CYCLOHEXANE	008C	016H			-453	936
GUANIDINIUM-5-NITRAMINOTETRAZO	002C	007H	0020	009N	58	937
LE					0	938
GUANIDINIUM NITRATE	001C	006H	0030	004N	-755	939
HEXANETRINITRATE	006C	011H	0090	003N	-420	940
HYDROXYLAMMONIUM NITRATE	004H	006O	003N		-843	941
HYDROXYLAMMONIUM PERCHLORATE	004H	005O	001CL		-496	942
HYDROXY TERMINATED POLYBUTADIE	567C,	006H	0010	004N	-116	943
NE NITRILE					0	944
HYDROGENATED HYDROXYTERMINATED	071C	120H	0027		-295	945
/POLYBUTADIENE					0	946
HYDROCARBON OIL	001C	002H			-756	947
HYDROXY TERMINATED POLYBUTADIE	073C	110H	0060		-30	948
NE					0	949
HYDROXYETHYLMETHACRYLATE	006C	010H	0030		-1153	950
ISOPROPYLAMMONIUM NITRATE	003C	010H	0030	002N	-813	951
ISODECYL PELARGONATE	019C	038H	0020		-714	952
LEAD-4,4-DIACETAMIDO SALICYLAT	018C	016H	0300	002N 001PB	-709	953
LOW ACETYL CELLULOSE ACETATE	428C	572H	2670		-1275	954
METHANOL	001C	004H	0010		-1773	955
METHOXY-DI-(BATOXYDIETHYLENE G	052C	111H	0160		-1229	956
LYCOL)					0	957
MELAMINE	006C	006H	006N		-165	958
MERCAPTO TERMINATED POLYBUTADI	699C	941H	0040	001S	47	959
ENE NITRILE					0	960
MONOMETHYLHYDRAZINE NITRATE	001C	007H	0030	003N	-565	961
N1,N1,O-TRIS(2-FLUORO-2,2-DINI	007C	006H	0140	007N 003F	-568	962
TROETHYL)-CARBAMATE					0	963
NITROSTARCH	600C	075H	1010	025N	-613	964
N-FLUORO-N-BUTYLNITRAMINE	004C	009H	0020	002N 001F	-288	965
N-FLUORO-SEC-BUTYLNITRAMINE	004C	009H	0020	002N 001F	-279	966
N-FLUORO-TERT-BUTYLNITRAMINE	004C	009H	0020	002N 001F	-225	967
N-BUTYL ACRYLATE	007C	012H	0020		-799	968
NONFUNCTIONAL POLYBUTADIENE	004C	006H			68	969
NONFUNCTIONAL POLYBUTADIENE	004C	006H			25	970
N,N,N'-TRIFLUOROHEXANEAMIDINE	006C	011H	002N	003F	-307	971
PETROLATUM(TECHNICAL)	071C	131H			-325	972
PETROLEUM JELLY	072C	130H			-161	973
PLASTICIZER(ESTER OF FATTY ACI	064C	126H	0060		-615	974
DS)					0	975
POLYETHYLENE (PELLETS)	002C	004H			-478	976
POLYETHYLENE (FILM)	002C	004H			-491	977
POLYETHYLEN GLYCOL	002C	004H	001O		-1059	978
POLYMETHYLENE POLYPHENYLISOCYA	015C	009H	001O	001N	-276	979
NATE					0	980
POLYOXYETHYLENE SORBITAN MONOL	050C	103H	0190		-1132	981
LAURCITE					0	982
POLYPROPYLENE FILM	003C	006H			-471	983
POLYETHYLENEAMMONIUM NITRATE	32?C	027H	1?90	151N	-675	984
POLYVINYLPYRROLIDINE	32.C	7 ?H	10?C	000N	-331	985
POLYPROPYLENE GLYCOL	030C	1 ?H	0170		-1?0?	0.301 986

POLYTETRAMETHYLENEETHER GLYCOL	C34O	114H	O15O			-516		989
POLY-1,4-BUTYLENE GLYCOL	C34O	114H	O15O			-751		990
POLYGLYCERYL OLEATE	C65O	O91H	14OO			10		989
POLYBUTENE-6	C72O	141H				-815		992
POLYBUTADIENE DIOL	C72O	110H	O99O			66		991
POLYBUTADIEN /ACRYLONITRILE	CO65?O	994H	O17O	O72N		514		992
POLYMER								993
POLYBUTADIENE/ACRYLONITRILE	CO654O	84?H	O84O	O89N		156		994
POLYMER						0		995
POLYBUTADIENE/ACRYLONITRILE	CO664O	83?H	O83O	O66N		138		996
POLYMER						0		997
PYROMELLITIC DIANHYDRIDE	C1?O	O?2H	OOCO			-1145		998
SORBITOL PENTANITRATE	?76O	O89N	O16O	O5?N		-463		999
TETRAMETHYLAMMONIUM NITRATE	2936	871H	2226	147N		-624		1000
TETRACYANOETHYLENE	66?O	O84N				1153		1001
TETRAETHYLAMMONIUM NITRATE	?87O	227H	OO2O	O62N		-602		1002
TRINITROFLUOROMETHANE	?81O	O?6O	OO2N	O31F		-311		1003
TRINITROCHLOROMETHANE	O61O	OO6O	O35N	O61CL		-35		1004
TRINITROBROMEMETHANE	O21O	O?69	O35N	O61BR		-14		1005
TRINITROMETHANE	?61O	O61H	O96O	O63N		-105		1006
TRIMETHYLAMMONIUM NITRATE	4936	O13H	OO3O	O62N		-673		1007
TRIETHYLENE GLYCOL DINITRATE	O3O6	O12H	OO5O	O?2N		-654		1008
TRIMETHYLOLPROPANE	O96O	O14H	O23O			-1339		1009
TRIETHYLAMINE	?26O	O15H	O91N			-490		1010
TRIETHYL CITRATE	5126	O2OH	O97O			-1291		1011
TRIS(1-(2-ETHYL)-AZIRIDINYL)PHOSPHINE OXIDE	C21O	O27H	O23O	O63N		-154		1012
						0		1013
TRINITROETHYLNITROXYETHYLNITRAMINE	C14O	O6OH	O11O	O6ON		-75		1014
						0		1015
STEAM	2H	1O				-3208		1016
FUG	?65N	14H	231O	5AR		-33		1017
PROPYLENE	3C	6H				116		1018
NITROGEN GAS	2N					0		1019
NIELSEN COMPOUND	17C	26H	4N			-164		1020
NO2 (GAS)	1N	2O				174		1021
IRON PENTACARBONYL	1FE	5C	5O			267		1022
RP-1 (RPL)	195H	1OOC				-361		1023
CESIUM NITRATE	1CS	1N	3O			-625	.1351	1024
TNT	7C	3N	6O	5H		79	.0597	1025
NOS365	52C	470H	7?OO	161N		-1421	.0560	1026
OTTO II	471C	676H	552O	155N		-696	.0452	1027
NOS 263	54C	459H	307O	159N		-1579	.0521	1028
OXSOL II	396H	4O4O	109N	65CL		-934	.0618	1029
OXSOL I	379H	4160	100N	79CL		-1061	.0618	1030
BROMINE (GAS)	2BR					46		1031
HYDROGEN BROMIDE (GAS)	1H	1BR				-103		1032
OTTO II	274C	526H	3?6O	94N		-696	.0452	1033
DECABORANE A	10B	16H	2N			-1198		1034
DECABORANE B	2CS	10B	13H			-624		1035
BITETRAZOLE	2C	8N	4H			797		1036
MOLYBDENUM TRIOXIDE	1MO	3O				-1253		1037
BROMOTRIFLUOROMETHANE	1C	1BR	3F			-1301		1038
TNENG	3C	6O	5H	7N		-63	.0704	1039
ETNEV	5C	13O	6H	5N		-187	.0675	1040
BENZOTRIFUROXANE (BTF)	6C	6O	6N			571	.0666	1041
AMMONIUM TRINITROIMIDAZOLE(AT	3C	6O	4H	6N		-16	.0662	1042
THICKOL TP-H-3314 (NO FE)	760H	3520	231O	105N	03CL 16S	-735	.0549	1043
AMMONIUM BIFLUORIDE(AF+LIW HF)	5N	1N	2F			-3139		1044
N2O4 (NTO MIL)	2N	4O				-51	.0517	1045
NORMAL HEXYL CARBORANE	8C	24H	10O			-394	.0379	1046
FC, POLYMER (O,NEILL)	9O	26C	1N	42H		-1275	.0619	1047
F17-47 (SIEG)	12C	5O	16H			-1290	.0444	1048
SYLGARD	1SI	1O	6H	2C		-1060		1049
WITCO F17-47 (JOS)	12C	5O	16H			-1310	.0430	1050
DIMER ACID/EPOXOL9S NEW DIMER	99C	174H	15O			-500	.0343	1051
R45 HTPB (UTC)	901H	0540	6O			5	.0336	1052

DI ISO CYANATE (DDI)	36C	72H	2N	2O		-354	.0319	1053
ISOBUTYLBENZENE	10C	14H				-124	.0313	1054
N,N DINITROSOPENTAMETHYLENETETRAMINE	5C	10H	6N	2O		369	.0545	1055
						0		1056
HYDRAZINE DIBORANE (JOS)	2B	10H	2N			-502	.0343	1057
HTPB/CURATIVE (JOS)	c56C	y7oH	5N	130		-493	.0329	1058
TRINITROETHYLORTHOCARBONATE	9C	8H	12N	2O		-257	.0304	1059
SHELL EPON 815	21C	24H	4O			-327	.0439	1060
ALUMINUM TRIOXIDE TRIHYDRATE	2AL	6O	6H			-3434	.0374	1061
LITHIUM PEROXIDE	2LI	2O				-2307	.0353	1062
AMMONIUM 5-NITRAMINOTETRAZOLE	1C	7N	5H	2O		222	.0536	1063
A TETRAZOLE POLYURETHANE	999H	523C	1230	243N		-399	.0419	1064
R45	661C	999H	1N	9O		40	.0325	1065
NGA (CT)	545C	946H	1590			-1086	.0379	1066
ZL 320	666C	969H	22N	90O		-579	.0373	1067
IPDI	12C	18H	2N	2O		-501	.0354	1068
ERL0510	15C	19H	1N	4O		-167	.0455	1069
CASTOR OIL	62C	111H	9O			-626	.0346	1070
AN	4H	2N	3O			-1085	.0623	1071
ADHG	149C	516H	214N	293O		-1272	.0623	1072
NG	1C	4H	4N	2O		-212	.0620	1073
TAGN	1C	9H	7N	3O		-84	.0569	1074
GN	1C	6H	4N	3O		-758	.0519	1075
GLYOXAL HYDRAZINE POLYMER	2C	2H	2N			278	.0356	1076
DHTT	4C	10H	16N			647	.0572	1077
HEXANITROBENZENE	6C	6N	12O			12	.0717	1078
MANGANESE	1MN					0	.2599	1079
PEG4000 (CARBOWAX)	2C	4H	1O			-1058	.0435	1080
BITRETRAZOLE	2C	2H	9N			725		1081
CHROMIUM CARBONYL JAX78/5168	1CR	6C	6O			-1170		1082
MOLYBDENUM CARBONYL JAX78/5168	1MO	6C	6O			-689		1083
TUNGSTEN CARBONYL JAX79/5168	1W	6C	6O			-645		1084
SODIUM AZIDE +TEFLON (STOICH)	1C	6N	2F	2NA		-478		1085
CATOCENE	27C	32H	2FE			115	.0414	1086
GE-RTV-615/A+B	2C	6H	1SI	1O		-1888	.0372	1087
HTPB (AFAPL VARIANT)	654C	988H	6N	20O		123	.0332	1088
CHROMIUM OCTOATE	1CR	24C	45H	6O		-506	.0361	1089
F1780	160C	255H	100O			-1297	.0433	1090
HMDI	8C	12H	2O	2N		-717	.0375	1091
HC434	669C	999H	1N	13O		-16	.0327	1092
MNA	7C	8H	2N	2O		-49	.0433	1093
MAR 658	40C	46H	8O			-696	.0419	1094
PCPO240	564C	999H	217O			-1393	.0395	1095
PCPO301	564C	999H	217O			-1393	.0396	1096
PAPI	224C	155H	27O	27N		-202	.0448	1097
POLYMEG 1000	4C	8H	1O			-874	.0355	1098
POLYMEG 2000	4C	8H	1O			-874	.0354	1099
POLYSTYRENE	8C	8H				106	.0379	1100
R-18	624C	999H	374O			-1364	.0326	1101
TATB	6C	6N	6O	6H		-143	.0698	1102
R45M	667C	999H	5O			-30	.0433	1103
STABOXOL P	13C	10H	2N			-41	.0379	1104
TEDGN	6C	12H	8O	2N		-645	.0480	1105
THERMAX	1C					0	.0704	1106
LACQUER NITROCELLULOSE	600C	774H	226N	952O		-663	.0599	1107
HYLENE W (DHF ESTIMATED)	15C	22H	2N	2O		-150	.0366	1108
C5H10N14O8 (NEED)	5C	10H	14N	8O		c479		1109
GLYCIDYL AZIDE	3C	7H	1O	3N		564	.0470	1110
LEAD STYPHNATE	1PB	6C	3H	3N	9O	-205	.1091	1111
CALCIUM CHROMATE	1CA	1CR	4O			-2111	.1044	1112
BARIUM CHROMATE	1BA	1CR	4O			-1347	.1625	1113

Appendix G

PEP AUXILIARY PROGRAM

In theory, the thermodynamic data for the combustion species could be put onto a magnetic tape and the SEARCH subroutine of the propellant program made to digest this information. In practice, it was decided to "predigest" this information with an auxiliary program, which is called PEPAUX. There are several reasons for this other than the fact that binary rather than a BCD tape may be produced. These will become apparent as the description progresses.

PEPAUX consists of a somewhat small program deck followed by two sets of input cards. The first set contains Holerith information and is somewhat permanent. Since this first may be considered part of the program deck, it will not be described in detail except to note that at present it contains 74 cards and that the first 47, which contain element names, may be permuted in any order. However, the order determines the precedence of the element in the molecular names. Hence, if H precedes C, methane will be denoted H4C; otherwise it will be denoted CH4. As can be suspected from this, PEPAUX generates automatically the Holerith names of all combustion species.

The second and main part of the input to PEPAUX is the thermodynamic data for the combustion species. This contains three card sets for as many species as desired. The first card is a species identification card, and the second two contain the data itself. The number of cards in this group is 3n + 1, where n is the number of species. An extra, blank card is placed at the end to signal the end of the input deck.

The identification card contains the molecular composition of the pertinent species and phase. The composition consists of as many information pairs as there are elements in the species. The information pairs begin in column 48 and repeat the format (A2,I2). The first part is the atomic symbol commonly used by chemists; the second is the number of such atoms in the molecules. For example, AL1CL3 designates $AlCl_3$. The phase of the species also appears on this card in column 36. Other information on this card, such as name and molecular weight, is not processed.

The two data cards which follow have a format compatible with the JANNAF thermochemical data in floating point form as follows:

FIRST CARD	L_1(end in 13) L_2(end in 26) L_3(end in 39) L_4(end in 52)
SECOND CARD	L_5(end in 13) L_6(end in 26) L_7(end in 39) L_8(end in 52)

where

$$C_p = L_1 + L_2\Theta + L_3\Theta^2 + L_4\Theta^3 + L_5\Theta^{-2}$$

L_6 is the integration constant for total enthalpy (kcal/mole)

L_7 is the integration constant for entropy (cal/mole/°K)

Θ is T/1000

(L_8 is the heat of formation and is not used.)

More thermodynamic data is permitted to follow the blank card. Another format is used for the second group of thermodynamic data, which is described in both NAVWEPS 7043 and NAVWEPS 7609. It will not be repeated here, especially since the JANAF fits have become generally accepted. Some remarks on PEPAUX operation follow.

PEPAUX not only generates Holerith names for each combustion species but also adds the symbol $ when the species is solid and the symbol * when it is liquid. Plus and minus signs are added for ionic species. However, only the leading six symbols are available on the output tape for the equilibrium program.

PEPAUX reorders the species so that gases come first, and condensed species follow on the output tape. This saves computing time when the equilibrium program utilizes this tape.

PEPAUX automatically deletes and edits. Species which are repeated are deleted and noted in the output. This provides a method of updating the thermo data files. Newer data is simply placed in front. This way, older data in back is deleted. If the input deck becomes too large, the redundant data can easily be removed by studying the previous PEPAUX output.

Logical tape 12 is written by PEPAUX and the plastic ring is removed. It is used by the equilibrium program until an updating effort is required of PEPAUX.

If one is using thermodynamic data supplied by NWC, the following peculiarities should be noted. The symbols U1, U2, U3, U4 and U5 are fictional elements that have the same data (except atomic number internally) as Be, B, Mg, Al, and C. Since only elementary species appear, this allows one to consider problems in which these elements do not burn. If one wants to know what happens if 10% of his aluminum does not burn, he inputs 90% of his aluminum as Al and 10% as U4.

The JANAF data was fit by Howard Shomate at NWC and supplied to Harold Prophet at Dow Chemical for further distribution. Shomate was not always satisfied with the fit and sometimes spliced two fits (over different temperature regimes) together. In these cases three groups of three cards appear for a single gaseous species. The first is the single fit and is ignored by PEPAUX, which picks up the better fit represented by the two regimes on the following six cards.

The PEPAUX program and input follow.

```
-ASG,AX CRUISE*PEPAUX//21734
-USE    12.,CRUISE*PEPAUX
-ASG,T A,F2///256
-USE 28,A
-ASG,T B,F2///256
-USE 29,B
-FOR,IS    PEPAUX,PEPAUX/A
      COMMON /PAUX/ JE(101), HI(101,2), IN(101), HK(50,2), KN(50), JN(7)
C UNIVAC 1108 VERSION, FORTRAN IV
     1,JE(7), OUT(22), SPEC(5), IS(5), PARA(20),REDUND(2,7777), JD, NJD
      INTEGER S
    1 FORMAT (14I3, 12X, I1, 15X, I1)                                          0070
    3 FORMAT (I2, 2A1, I1)                                                     0090
    4 FORMAT (2A1,I1)                                                          0100
    5 FORMAT (A1,I1)                                                           0110
    8 FORMAT (I8, 2A6, I6)
    9 FORMAT (1H 3I5, 2X, A6)                                                  0150
  554 FORMAT (7(F3.0,1X,A6), I2/  E12.0,F6.0,E12.0)
   10 FORMAT (15HREDUNDANCY IN 2A6)
      REWIND 28
      REWIND 29
      DO 11  I = 1,97
   11 READ  (5,3)JE(I), HI(I,1), HI(I,2), IN(I)                               0190
      DO 12  I = 1,22                                                          0200
   12 READ  (5,4)HK(I,1), HK(I,2), KN(I)                                       0210
      DO 13  I = 1,5                                                           0220
   13 READ  (5,5)SPEC(I), IS(I)                                                0230
      CALL BUFFER (1,0,0,0.,0,0,0.)
      HI(98,1) = SPEC(4)
      HI(99,1) = SPEC(5)
      HI(98,2) = HK(I,1)
      HI(99,2) = HK(I,1)
      CALL SHOJAN
      CALL NONJAN
      LIM = JD + NJD
      DO 110  K = 1,2                                                          0730
      REWIND 28
      REWIND 29
      DO 108  I = 1,LIM                                                        0750
      READ (29,8)    KHASE,          REDUND(1,I), REDUND(2,I),S
      READ (28) (JJ(L), JE(L), L = 1,7)
  102 READ (28) (PARA(L), L = 1,9)
  103 READ (28) (PARA(L), L = 10,18)
      WRITE (6,6666) KHASE, REDUND(1,I), REDUND(2,I), (JN(L), JE(L),
     1 L = 1,7), (PARA(L), L = 1,18),S
 6666 FORMAT (I5, 2A6, 9X, 14I3/ 9E13.4/9E13.4,I5)
      IF (I .LE. JD) GO TO 107
      IF (K .EQ. 2)  GO TO 107
  104 LII = I-1                                                                0820
      IF (JE(1) .EQ. 55)  GO TO 107
      DO 105  J = 1,LII                                                        0830
      IF (REDUND(1,J) - REDUND(1,I))  105,106,105                              0840
  106 IF (REDUND(2,J) - REDUND(2,I))  105,109,105                              0850
  105 CONTINUE                                                                 0860
  107 GO TO (50,55), K                                                         0870
   50 IF (KHASE - 1)  108,51,108                                               0880
   51 CALL BUFFER (2,KHASE,S,REDUND(1,I), JN, JE, PARA)
      GO TO 108                                                                0950
   55 IF (KHASE-1)  108,108,51                                                 0960
  109 WRITE (6,10)REDUND(1,I), REDUND(2,I)                                     0970
  108 CONTINUE                                                                 0980
  110 CONTINUE                                                                 0990
      KHASE = -1
      CALL BUFFER (3,KHASE,S,REDUND(1,I), JN, JE, PARA)
      CALL KINDAT
      END FILE 12
```

```
      REWIND 12
      WRITE (6,6420)
 6420 FORMAT (29H1 PEPAUX WORKED SUCCESSFULLY.)
      CALL EXIT                                                          1040
      END                                                                1050
-FOR,IS   SHOJAN,SHOJAN/A
      SUBROUTINE SHOJAN
C . . . . SUBROUTINE TO DIGEST JANAF DATA AS FITTED BY HOWARD SHOMATE.
      COMMON /PAUX/ IE(101), HI(101,2), IN(101), HK(50,2), KN(50), JN(7)
     1,JE(7), OUT(22), SPEC(5), IS(5), PARA(20),REDUND(2,7777), JD, NJD
      DIMENSION CRAZE(3)
      DATA (CRAZE(I), I = 1,3)/ 1HC, 1HG, 1HL /
      DIMENSION HOL(5), ELM(6,2), NA(6)
      INTEGER S,SA
    1 FORMAT (5A6, 5X, A1, 11X, 6(2A1, I2), 1X, I6)
    2 FORMAT (I8, 12A1, I6)
    3 FORMAT (4(F13.0), F5.0, 3X, F5.0, 8X, I5)
    4 FORMAT (7H0MIX UP  219)
      JD = 0
      JN(7) =  0
  101 READ (5,1) (HOL(I),I=1,5), PHASE, ((ELM(I,J),J=1,2),NA(I),I=1,6),S
  102 IFIRST = 0
  103 DO 11  I = 1,18
   11 OUT(I) = SPEC(1)
      IF (NA(1) .EQ. 0)  RETURN
C . . . . IF NO ATOM COUNT, SHOJAN IS FINIISHED.
      JD = JD + 1
      INDEX = 1
      DO 9  I = 1,7
      JN(I) = 0.
    9 JE(I) = 0.
      DO 17  I = 1,99
      DO 16  J = 1,6
C . . . . COMPARE HOLERITH WITH PERIODIC TABLE.
      IF (HI(I,1) .NE. ELM(J,1))  GO TO 16
      K = NA(J)
      IF (I .GE. 98)  GO TO  12
      IF (HI(I,2) .NE. ELM(J,2))  GO TO 16
      OUT(INDEX) = HI(I,1)
      OUT(INDEX+1) = HI(I,2)
      INDEX = INDEX + IN(I)
      OUT(INDEX) = HK(K,1)
      OUT(INDEX+1) = HK(K,2)
      INDEX = INDEX + KN(K)
      JN(J) = K
      JE(J) = IE(I)
      GO TO 17
C . . . . ATTACH CHARGE APPENDAGES.
   12 DO 13  L = 1,K
      OUT(INDEX) = ELM(J,1)
   13 INDEX = INDEX + 1
      JN(J) = K
      JE(J) = 0
      IF (I .EQ. 98) JN(J) = -K
      GO TO 17
   16 CONTINUE
   17 CONTINUE
      IF (JE(1) .NE. 0)  GO TO 18
      OUT(2) = OUT(1)
      OUT(1) = 1HE
C . . . . ATTACH PHASE IDENTIFICATION APPENDAGE.
   18 KHASE = 2
      IF (PHASE .EQ. CRAZE(1))  OUT(INDEX) = SPEC(2)
      IF (PHASE .EQ. CRAZE(2))  KHASE = 1
      IF (PHASE .EQ. CRAZE(3))  OUT(INDEX) = SPEC(3)
      WRITE (29,2) KHASE, (OUT(I), I = 1,12), S
```

```
      WRITE (28) (JN(L), JE(L), L = 1,7)
   87 READ (5,3) A,B,C,D,TL,TU,SA
      IF (S .NE. SA)  WRITE (6,4) S,SA
      READ (5,3) E,F,G,H,TL,TU,SA
      IF (S .NE. SA)  WRITE (6,4) S,SA
      READ (5,1) (HOL(I),I=1,5), PHASE, ((ELM(I,J),J=1,2),NA(I),I=1,6),S
      IF (S .NE. SA)   GO TO 89
      IF (PHASE .NE. CRAZE(2))  GO TO 89
      IF (IFIRST .NE. 0)  GO TO 88
      IFIRST = 1
      GO TO 87
   88 WRITE (28) A,B,C,D,E,F,G,TL,TU
      READ (5,3) A,B,C,D,TL,TU,SA
      IF (S .NE. SA)  WRITE (6,4) S,SA
      READ (5,3) E,F,G,H,TL,TU,SA
      IF (S .NE. SA)  WRITE (6,4) S,SA
      WRITE (28) A,B,C,D,E,F,G,TL,TU
      GO TO 101
   89 WRITE (28) A,B,C,D,E,F,G,TL,TU
      WRITE (28) A,B,C,D,E,F,G,TL,TU
      GO TO 102
      END
-FOR,IS   CONVER,CONVER/A
      SUBROUTINE CONVER (PARA, A,B,C,D,E,F,G,TL,TU)
C . . . . SUBROUTINE TO CONVERT OLD PARAMETRIC FORMS TO NEW PARAMETRIC FORMS.
      DIMENSION PARA(20)
      A = PARA(3)
      B = PARA(4)*1000.
      C = 0.
      D = 0.
      E = PARA(5)/1000000.
      F = PARA(1) + PARA(2) - PARA(3)*3000. - PARA(4)*4500000.
     1    + PARA(5)/3000.
      F = F/1000.
      G = PARA(6) - PARA(3)*ALOG(3000.) - PARA(4)*3000.
     1   + PARA(5)/4500000. + ALOG(1000.)
      TL = PARA(7)
      TU = PARA(8)
      RETURN
      END
-FOR,IS   NONJAN,NONJAN/A
      SUBROUTINE NONJAN
C . . . . THIS SUBROUTINE PROCESSES NON JANAF TYPE DATA ACCORDING TO DOW
C . . . . AND OLD NOTS (NAVWEPS 7043) FORMATS.
      COMMON /PAUX/ IE(101), HI(101,2), IN(101), HK(50,2), KN(50), JN(7)
     1,JE(7), OUT(22), SPEC(5), IS(5), PARA(20),REDUND(2,7777), JD, NJD
      DATA  ELECT/ 6HEEEEEE /
    1 FORMAT (14I3, 12X, I1, 15X, I1)
    2 FORMAT (I8, 12A1, I6)
    6 FORMAT (4E13.0)                                                    0120
    7 FORMAT (6E9.6,2F6.0,I1)                                            0130
      NJD = 0
      DO 99  LIM = 1,7777                                                0240
      DO 98 I = 1,18                                                     0250
   98 OUT(I) = SPEC(1)                                                   0260
      READ  (5,1)(JN(I), JE(I), I = 1,7), LEVEL,KHASE                    0270
      IF (JN(1) .EQ. 0)  GO TO 100
C . . . . IF NO ATOM COUNT,SKIP OUT.
      NJD = NJD + 1
   29 IF (KHASE)  30,31,30                                               0290
   30 READ (5,6) A, B, C, D, E, F, G
      TL = 298.
      TU = 6000.
      JAN = 1                                                            0310
      GO TO 32                                                           0320
   31 READ  (5,7)(PARA(I), I = 1,8),KHASE,(PARA(I),I = 9,16)             0330
```

```
      JAN = 2                                                          0340
   32 INDEX = 1
      DO 17  I = 1,97
      DO 16  J = 1,7                                                   0370
      KK = J
      IF (JN(J))  14,17,14                                             0380
   14 IF (IE(I) - JE(J))  16,15,16                                     0390
   15 OUT(INDEX) = HI(I,1)                                             0400
      OUT(INDEX+1) = HI(I,2)                                           0410
      INDEX = INDEX + IN(I)                                            0420
      K = JN(J)                                                        0430
      OUT(INDEX) =HK(K,1)                                              0440
      OUT(INDEX+1) = HK(K,2)                                           0450
      INDEX = INDEX + KN(K)                                            0460
      GO TO 17                                                         0470
   16 CONTINUE                                                         0480
   17 CONTINUE                                                         0490
      OUT(INDEX) = SPEC(KHASE)                                         0500
      INDEX = INDEX + IS(KHASE)                                        0510
      IF (JE(1) .NE. 0)  GO TO 23
      IF (INDEX .NE. 1)  GO TO 18
      OUT(INDEX) = ELECT
      INDEX = 2
   18 IAB = ABS(JN(1))                                                 0530
      IF (JN(1))  19,23,21                                             0540
   19 DO 20  I = 1,IAB                                                 0550
      OUT(INDEX) = SPEC(4)                                             0560
   20 INDEX = INDEX + IS(4)                                            0570
      GO TO 23                                                         0580
   21 DO 22  I = 1,IAB                                                 0590
      OUT(INDEX) = SPEC(5)                                             0600
   22 INDEX = INDEX + IS(5)                                            0610
   23 IL = MIN0(INDEX-6,6)                                             0620
      IL = 1
      IU = IL + 11                                                     0630
      WRITE (29,2) KHASE, (OUT(I), I = IL,IU), NJD
      WRITE(28) (JN(L), JE(L), L = 1,7)
      IF (JAN .EQ. 2)  CALL CONVER (PARA(1),A,B,C,D,E,F,G,TL,TU)
      WRITE (28) A,B,C,D,E,F,G,TL,TU
      IF (JAN .EQ. 2)  CALL CONVER (PARA(9),A,B,C,D,E,F,G,TL,TU)
      WRITE (28) A,B,C,D,E,F,G,TL,TU
   99 CONTINUE
  100 RETURN
      END
-FOR,IS   KINDAT,KINDAT/A
      SUBROUTINE KINDAT
C . . . . THIS SUBROUTINE READS IN CHEMICAL KINETIC AND COLLISION CROSS
C . . . . SECTION DATA FOR MORE ADVANCED VERSIONS OF THE THERMOCHEMICAL
C . . . . PROGRAM.
      DIMENSION PARA(20)
      REAL JUMP
  554 FORMAT (7(F3.0,1X,A6), I2/  E12.0,F6.0,E12.0)
      DO 209  I = 1,1000
      READ (5,554) (PARA(K), K = 1,14),LBJ,BUMP,JUMP,HUMP
      IF (LBJ .NE. 1)  GO TO 556
      BUMP = -BUMP
  556 WRITE (12) (PARA(K), K = 1,14) , BUMP, HUMP, JUMP
      IF (PARA(1) .EQ. 0.)  GO TO 210
  209 CONTINUE
  210 CONTINUE
      DO 219  I = 1,1000
      READ (5,555)  VA, VB, VC
      WRITE (12) VA, VB, VC
      IF (VA .EQ. 3.) GO TO 220
  219 CONTINUE
  220 CONTINUE
```

```
  555 FORMAT (F4.0, A6, E10.0)
      RETURN
      END
-FOR,IS   BUFFER,BUFFER/A
      SUBROUTINE BUFFER (IW, PHASE, S, REDUND, JN,JE, PARA)
      DIMENSION BIN(20,35), JE(7), JN(7), PARA(18)
      IF (IW.EQ. 1)  GO TO 11
      I=I+1
      BIN(I,1) = PHASE
      GO TO(11,21,51), IW
   11 REWIND 12
      I = 0
      GO TO 99
   21 BIN(I,2) = REDUND
      BIN(I,3) = S
      DO 31  J = 1,7
      K = 3 + 2*(J-1)
      BIN(I,K+1) = JN(J)
   31 BIN(I,K+2) = JE(J)
      DO 41  J = 1,18
   41 BIN(I,J+17) = PARA(J)
      IF (PHASE .LT. 0.)  GO TO 51
      IF (I .LT. 20)  GO TO 99
      I = 0
   51 WRITE (12) ((BIN(J,K), K = 1,35), J = 1,20)
   99 RETURN
      END
-XQT
 3LI2
11NA2
19K 1
37RB2
55CS2
87FR2
 4BE2
12MG2
20CA2
38SR2
56BA2
88RA2
 5B 1
13AL2
21SC2
39Y 1
57LA2
89AC2
95U52
96U12
97U22
98U32
99U42
22TI2
23V 1
24CR2
25MN2
26FE2
27CO2
28NI2
29CU2
30ZN2
31GA2
32GE2
40ZR2
41CB2
42MO2
43TC2
```

```
44RU2
45RH2
46PD2
47AG2
48CD2
49IN2
50SN2
58CE2
59PR2
60ND2
61PM2
62SM2
63EU2
64GD2
65TB2
66DY2
67HO2
68ER2
69TU2
70YB2
71LU2
72HF2
73TA2
74W 1
75RE2
76OS2
77IR2
78PT2
79AU2
80HG2
81TL2
82PB2
90TH2
91PA2
92U 1
93NP2
14SI2
 6C 1
83BI2
51SB2
33AS2
15P 1
 7N 1
 1H 1
84PO2
52TE2
34SE2
16S 1
 8O 1
85AT2
53I 1
35BR2
17CL2
 9F 1
 2HE2
10NE2
18AR2
36KR2
54XE2
  0
2 1
3 1
4 1
5 1
6 1
7 1
```

```
8 1
9 1
102
112
122
132
142
152
162
172
182
192
202
212
222
 0
$1
*1
+1
-1
 ALUMINUM                              (C)   26.982 AL 1                                          2-A
 .79604324E+1-.74234602E+1 .12013784E+2-.41592804E+1  298 TO 0932    1265     2-B
-.79464640E-1-.24076189E+1 .17672812E+2 .00000000     298 TO 0932    1265     2-C
 ALUMINUM                              (C)   26.982 U4 1                                          2-D
 .79604320+01-.74234596+01 .12013784+02-.41592802+01  298 TO 0932    1265     2-E
-.79464629-01-.24076188+01 .17672811+02 .00000000     298 TO 0932    1265     2-F
 ALUMINUM, MONATOMIC                   (G)   26.982 AL 1                                          4-A
 .48557431+01 .17986383-00-.84569434-01 .12009095-01  298 TO 6000    1265     4-B
 .19636010-01 .76611834+02 .45244449+02 .77999999+02  298 TO 6000    1265     4-C
 ALUMINUM  MONOCHLORIDE                (G)   62.435 AL 1CL 1                                      6-A
 .88697597+01 .17984430-00-.16823909-01 .14357672-02  298 TO 6000     964     6-B
-.57386842-01-.14046012+02 .64827267+02-.11200000+02  298 TO 6000     964     6-C
 ALUMINUM                              (L)   26.982 AL 1                                          3-D
 .75878742+01 .11669338-03-.29586136-04 .21870895-05 0932 TO 6000    1265     3-B
 .93873461-05-.19028412-00 .17602579+02 .20720000+01 0932 TO 6000    1265     3-C
 ALUMINUM                              (L)   26.982 U4 1                                          3-D
 .75878742+01 .11669338-03-.29586136-04 .21870895-05 0932 TO 6000    1265     3-E
 .93873461-05-.19028412-00 .17602579+02 .20720000+01 0932 TO 6000    1265     3-F
 ALUMINUM, MONATOMIC                   (G)   26.982 U4 1                                          4-A
 .48557431+01 .17986383-00-.84569434-01 .12009095-01  298 TO 6000    1265     4-B
 .19636010-01 .76611834+02 .45244449+02 .77999999+02  298 TO 6000    1265     4-C
 ALUMINUM  CHLOROFLUORIDE              (G)   81.433 AL 1CL 1F  1                                   7-A
 .13469642+02 .37285351-00-.10065834+00 .85780834-02  298 TO 6000     964     7-B
-.18165674-00-.12464722+03 .82534085+02-.12000000+03  298 TO 6000     964     7-C
```

Appendix H

LISTING OF PEP PROGRAM

```
      SUBROUTINE ADJUST
COMMENT.   ADJUSTS GRAM ATOM BALANCE ERRORS BY MODIFYING THE BASIS.
CALLED BY DEFIOJ
     0COMMON A(12,12), WR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,6), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(200), W47, NAME, SER
     0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SD(200), V(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), PA(200,2), RR(200,2), PC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      DIMENSION EP(12), X(12)
      DO 1  I = 1,IS
      EP(I) = ALP(I)
      DO 1  J = 1,N
    1 EP(I) = EP(I) - C(I,J)*VNT(J)
      DO 2  K = 1,IS
      X(K) = 0.
      DO 2  I = 1,IS
    2 X(K) = X(K) + A(I,K)*EP(I)
      DO 3  K = 1,IS
      J = IOJ(K)
    3 VNT(J) = VNT(J) + X(K)
   77 FORMAT (1P 12E10.2)
      IF (WR(16) .EQ. 0)  GO TO 99
      WRITE (6,77) (ALP(J), J = 1,IS)
      WRITE (6,77) ( EP(J), J = 1,IS)
      WRITE (6,77) (X(J) , J = 1,IS)
   99 RETURN
      END



      SUBROUTINE BOOST(W43,SSI)
COMMENT.   COMPUTES DRAG FREE BOOST VELOCITIES FROM IMPULSE AND DENSITY.
C     IF NOT DESITED, DELETE THE CALL IN SUBROUTINE DESIGN.
      DIMENSION W42(20), W44(20)
      DATA JM/18 /
      DATA(W42(I), I = 1,18)/5.,10.,15.,25.,30.,55.,60.,69.,71.,88.,
     1  100.,150.,175.,200.,300.,1000.,3000.,5000. /
227   FORMAT(/6(F5.0,1H/F6.0)/6(F5.0,1H/F6.0)/6(F6.0,1H/F5.0))
  230 FORMAT(/43HOBOOST VELOCITIES FOR PROPELLANT DENSITY OF F8.5,
     110H  (S.G. OF F8.3, 1H))
      W48 = 1728.*W43
  123 V0 = W43/.036128
      VI = SSI*32.174
      DO 127 J = 1, JM
  127 W44(J) = VI*ALOG(1.0+ W48/ W42(J))
  138 WRITE (6,230) W43, V0
      WRITE (6,227)(W42(J), W44(J), J=1,JM)
  139 RETURN
      END
```

```
      SUBROUTINE DEFIOJ
C     COMPUTES SERIAL NUMBER FOR AN OPTIMUM BASIS A LA HN BROWNE JR.
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SU(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     4,LL(200)
      CALL SLITET(1,KOOOFX)
       GO TO(7,11),KOOOFX
    7 CALL SLITE (1)
      CALL RANK(IR,W3,N)
      DO 1  I = 1,N
    1 LL(I) = 9
    2 IF = 0
      DO 6  I = 1,IS
    3 IF = IF + 1
      IF (IF-N)  9,9,8
    8 WRITE (6,10)
   10 FORMAT (17HOCANT FIND BASIS  )
      CALL EXIT
    9 DO 4  J = 1,IS
      K = IR(IF,1)
    4 A(J,I) = C(J,K)
    5 CALL LINDEP(I)
      CALL SLITET(2,KOOOFX)
      GO TO (66,3), KOOOFX
   66 LL(K) = 0
    6 IOJ(I) = K
      CALL ADJUST
   11 RETURN
      END
```

```
      SUBROUTINE DESIGN (TE,PR,HE,SYSENT,J,I)
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(97), W47, NAME, SER
      COMMON /SCRATC/PLOT(5,100)
     0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SU(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      DIMENSION TEMP(20),PRES(20),HEAT(20),VOLU(20),IPH(20)
      DIMENSION SPI(2),AST(2),PST(2),GAM(2),CF(2),EV(2),CST(2),RISP(2),
     1OEX(2),EL(2),THRT(2),TEX(2)
    1 FORMAT (4E16.6, I9)
      TEMP(I) = TE
      PRES(I) = PP
      HEAT(I) = HE
      VOLU(I) = FN*.08205*TE/PR
      IPH(I) = IPHASE(J)
      NPNTS = I
      IF (I.EQ. 1)  GO TO 99
      SPI(J+1) = 9.3294*SQRT((HEAT(1)-HEAT(2))/W27)
```

```
 10 TEX(J+1) = TEMP(2)
    AS = VOLU(2)/SQRT(HEAT(1)-HEAT(2))
    CONV = 1./1000./SQRT(8372.*W27)
    NSTART = 2
    IF (J .EQ. 0)  GO TO 21
    DO 20  LIM = 1,8
    DO 19  K = NSTART, NPNTS
    IF (NPNTS .EQ. 2)  GO TO 9
    IF (IPH(K-1) .EQ. IPH(K))  GO TO 19
    IF (ABS(TEMP(K)-TEMP(K-1)) .LT. 2.) GO TO 19
  9 TEMP(K+1) = TEMP(K)
    PRES(K+1) = PRES(K)
    HEAT(K+1) = HEAT(K)
    IPH(K+1) = IPH(K)
    VOLU(K+1) = VOLU(K)
    IPH(K) = IPH(K-1)
    NSTART = K+1
    NPNTS = NPNTS + 1
    TUP = TEMP(K-1)
    TLO = TEMP(K+1)
    PUP = PRES(K-1)
    PLO = PRES(K+1)
    HUP = HEAT(K-1)
    HLO=HEAT(K+1)
    DO 15  L = 1,10
    TEMP(K) = .5*(TUP+TLO)
    TE = TEMP(K)
    IF (TE +1. .LT. TEMP(1))  GO TO 151
    TEMP(K) = TLO
    PRES(K) = PLO
    HEAT(K) = HLO
    GO TO 16
151 IF (TE -1.  .GT. TEX(2))  GO TO 152
    TEMP(K) =TUP
    PRES(K) =PUP
    HEAT(K) =HUP
    VOLU(K) = FN*.08205*TEMP(K)/PRES(K)
    GO TO 21
152 TE=TEMP(K)
    CALL TSBAL (TE, PRES(K), HEAT(K), SYSENT,PUP,PLO)
    IVA = IPHASE(J)
    IF (IVA .NE. IPH(K-1))  GO TO 13
    IF (IVA .EQ. IPH(K+1))  GO TO 16
    TUP = TEMP(K)
    PUP = PRES(K)
    HUP = HEAT(K)
    GO TO 15
 13 TLO = TEMP(K)
    PLO = PRES(K)
    HLO = HEAT(K)
    IPH(K) = IVA
 15 CONTINUE
 16 VOLU(K) = FN*.08205*TEMP(K)/PRES(K)
    GO TO 20
 19 CONTINUE
    GO TO 21
 20 CONTINUE
 21 DO 31  L = 2,NPNTS
    CALL ONE D(HEAT(1),TEMP(L-1),PRES(L-1),HEAT(L-1),VOLU(L-1),TEMP(L)
   1,PRES(L), HEAT(L), VOLU(L), PST(J+1), ASTAR,    GT, GC, GV, LL)
    IF (PRES(L) .LT. PST(J+1))  GO TO 53
 31 CONTINUE
 53 IF (PST(J+1) .LT. PRES(L-1))  GO TO 32
    PST(J+1) = PRES(L-1)
    ASTAR = VOLU(L-1)/SQRT(HEAT(1) - HEAT(L-1))
```

```
   32 OEX(J+1) = AS/ASTAR
      GAM(J+1) = GV
      CONV = 1./1000./SQRT(9368.*W27)
      AST(J+1) = ASTAR*CONV
      CONV1 = 9.806/1000./4184./24.218
      CF(J+1) = CONV1*SPI(J+1)/W1(5)/AST(J+1)
      EV(J+1) = 32.174*SPI(J+1)
      RISP(J+1) = W43/.03613 *SPI(J+1)
      EL(J+1) = (W43/.03613)**(.78)    *SPI(J+1)
      AST(J+1) = AST(J+1)*1550./.00220462
      THRT(J+1) = TEMP(L)*(PRES(L)/PST(J+1))**GT
      IF (J .EQ. 0)  GO TO 99
      CONV = CONV/CONV1
      PAST = PST(J+1)
 9875 DO 49  K = 1,100
      IF (KR(3) .NE. 0  .AND.  K .EQ. 2) GOTO9876
      PLOT(1,K) = K
      AREA = ASTAR*PLOT(1,K)
      DO 33 M = L,NPNTS
      IF (M .GE. NPNTS)  GO TO 34
      IF (AREA .LT. VOLU(M)/SQRT(HEAT(1) -HEAT(M)))  GO TO 34
   33 CALL ONE D(HEAT(1),TEMP(M+1),PRES(M+1),HEAT(M+1),VOLU(M+1),TEMP(M)
     1,PRES(M),HEAT(M),VOLU(M),VA,VB,GT,GC,GV,LL)
   34 L = M
      PUP = PAST
      PLO = PAST/3.
      DO 43  M = 1,28
      PLOT(2,K) = .5*(PUP+PLO)
      IF ((PUP-PLOT(2,K))*(PLO-PLOT(2,K)))  35,44,44
   35 VOL = VOLU(L)*(PRES(L)/PLOT(2,K))**(1./GV)
      GO TO (36,37), LL
   36 HE = HEAT(L) + GC*(VOL*PLOT(2,K) - PRES(L)*VOLU(L))
      GO TO 38
   37 HE = HEAT(L) + GC*ALOG(PLOT(2,K)/PRES(L))
   38 IF (AREA    VOL/SQRT(HEAT(1)-HE))  39,44,40
   39 PLO = PLOT(2,K)
      GO TO 43
   40 PUP = PLOT(2,K)
   43 CONTINUE
   44 PAST = PLOT(2,K)
      PLOT(3,K) = TEMP(L)*(PRES(L)/PLOT(2,K))**GT
      PLOT(4,K) = 9.3294*SQRT((HEAT(1)-HE)/W27)
      PLOT(5,K) = PLOT(4,K) + PLOT(2,K)*AREA*CONV
   49 CONTINUE
    2 FORMAT (1P 5E18.7)
 9876 WRITE (6,1243)
 1243 FORMAT(/   72HOIMPULSE  IS EX      T*      P*      CF    ISP*  OPT EX
     X D-ISP    A*M.    EX T)
 1245 FORMAT( F7.1,F8.4,F7.0,F7.2,F7.3,F7.1,F7.2,F7.1,F8.5,F7.0)
 1244 FORMAT(/F7.1,F8.4,F7.0,F7.2,F7.3,  7X,F7.2,F7.1,F8.5,F7.0)
      WRITE( 6,1244)SPI(1),GAM(1),THRT(1),PST(1),CF(1),       OEX(1)
     1    , RISP(1), AST(1), TEX(1)
      CST(2) = PLOT(5,1)
      WRITE(6,1245) SPI(2),GAM(2),THRT(2),PST(2),CF(2),CST(2),OEX(2)
     X,RISP(2),AST(2),TEX(2)
   24 FORMAT('0INGRED. DENSITIES ARE'/(9F8.4))
      WRITE(6,24)(RHO(I),I=1,IN)
      IF(KR(3) .GT. 0)GO TO 98
C DELETABLE NON- ASCII OUTPUT OF DATE AND TOFDAY.
      WRITE(6,23)(ISERI(I),I=2,6)
   23 FORMAT('1',5A6)
      CALL BOOST(W43,SPI(2))
   98 CONTINUE
   99 RETURN
      END
```

```
      SUBROUTINE DESNOZ
C    NOZZLE HARDWARE DESIGN ROUTINE.
      DCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      COMMON /SCRATC/PLOT(5,100)
      CALL SLITET(3,ISC)
      IF (ISC .EQ. 1)  GO TO 99
   23 FORMAT('1',5A6)
      DO 49 K=1,100
      TVA=PLOT(4,K)+(PLOT(5,K)-PLOT(4,K))*(PLOT(2,K)-1.)/PLOT(2,K)
      IF(K .EQ. 26  .OR.  K .EQ. 66)WRITE(6,23)(ISERI(I),I=2,6)
      IF (K .EQ. 1  .OR.  K .EQ. 26  .OR.  K .EQ. 66)WRITE(6,2000)
2000  FORMAT('0',' EXP.',' EXIT',' EXIT',' EXIT',' OPTIMUM'
     &,' OPTIMUM',' VACUUM',' VACUUM',' SEA LV',' SEA LV'/
     $' RATIO',' PRESS',' PRESS',' TEMP',' IMPULSE',' IMPULSE'
     &,' IMPULS',' IMPULS',' IMPULS',' IMPULS'/
     &1DX,'ATM',' SI',' K',' SEC',' SI',' SEC'
     &,' SI',' SEC',' SI')
      VA=PLOT(2,K)*1001.3
      VB=PLOT(4,K)*9.80621
      VC=PLOT(5,K)*9.80621
      VD=TVA*9.90621
49    WRITE(6,7777)PLOT(1,K),PLOT(2,K),VA,PLOT(3,K),PLOT(4,K),VB,
     &PLOT(5,K),VC,TVA,VD
7777  FORMAT(F6.0,F7.3,F7.1,F7.0,F8.1,F8.0,F7.1,F7.0,F7.1,F7.0)
   99 RETURN
      END
```

```
      SUBROUTINE EQUIL(TE,PR,HE,ENTR,IX)
COMMENT.   THIS ROUTINE COMPUTES CHEMICAL EQUILIBRIUM FOR A PRESSURE,
C    TEMPERATURE POINT.   OTHER OUTPUTS ARE ENTHALPY AND ENTROPY.   HEAT
C     (CP) AND MOLES OF GAS ARE AVAILABLE THRU COMMON.
C    THIS ROUTINE IS CALLED BY PEP, HBAL, SBAL, AND TSBAL.
COMMENT    UNITS ARE TE (DEG. K.) PR (ATM.) HE (CAL/SYS WT.) ENTR (CAL/D
C      /SYS. WT.)           SYSTEM WEIGHT IS W27 IN COMMON.
COMMENT.   IX IS 0 FOR FROZEN EVALUATION OF THERMODYNAMIC VARIABLES.
C      IX IS 1 FOR EQUILIBRIUM EVALUATIONS (IX = 2 FOR KINETIC IN SOME VER
COMMENT.  IN ADDITION TO PRESSURE TEMPERATURE POINTS THIS ROUTINE MAY BE
C     FREELY FOR VOLUME TEMPERATURE POINTS BY USING THE FOLLOWING MODIFIE
C     CALL SEQUENCE. VNT(NP)=ALOG(.08205*TE/V))   KR(17) = 1      CALL EQU
C     (TE, PR, HE, ENTR, IX)          KR(17) = 0      PR=FN*VNT(NP)
C    V IS THE SYSTEM VOLUME IN LITERS/SYS. WT.
      DCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      DCOMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      COMMON/MOON/TSTEST
      DIMENSION X(12), XM(12)
    8 FORMAT (I5,F10.0, F12.3)
    9 FORMAT (1P 10E13.4)
 1734 CALL GIBBS(TE)
      CALL FIXBAS
 1735 IF (IX - 1)  21,12,12
   12 DO 38  J = 1,IS
      X(J) = 0.
      XM(J) = 0.
      DO 31  I = 1,N
      IF (C(J,I) .EQ. 0.)  GO TO 31
      XM(J) = AMAX1(VNT(I), XM(J))
      X(J) = X(J) + C(J,I)*VNT(I)
```

```
 31 CONTINUE
    IF (ABS(ALP(J) - X(J))/XM(J) .LT. .00001)  GO TO 38
    CALL SLITE(1)
    GO TO 39
 38 CONTINUE
 39 CALL DEFIOJ
    CALL REACT (TE)
    DO 211  I = 1,N
211 W3(I) = 50.0 -VLNK(I)
    CALL RANK(IR,W3,N)
 11 DO 22  JC = 1,20
    CALL TWITCH(PR,0)
    CALL SLITET(4,KOOOFX)
     GO TO(146,17),KOOOFX
146 IF (KR(13)-1)  15,14,15
 14 WRITE (6,8)JC,TE,PR
    WRITE (6,9)(VNT(I), I = 1,N)
 15 DO 23  ICC = 1,3
 25 CALL TWITCH(PR,1)
    CALL SLITET(4,KOOOFX)
     GO TO(24,22),KOOOFX
 23 CONTINUE
 22 CONTINUE
    CALL SLITE (3)
 21 VNT(NP) = ALOG(PR/FN)
 17 CALL THERMO (TE, HE, ENTR)
    VNT(NP) = EXP(VNT(NP))
    TET = TE
    RETURN
    END

    SUBROUTINE FIXBAS
   0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
   1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
   2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
   0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
   1TAU, H(200), S0(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
   2IOJ(12), PA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
   3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
   4,LL(200)
    IF (IG .EQ. N)  GO TO 99
    IGP = IG+1
    DO 9  J = 1,IS
    II = IOJ(J)
    IF (DMU(II) .LT. .9E+12)  GO TO 9
    DO 8  I = IGP,N
    IQ = 99
    IF (VNU(I,J) .EQ. 0.)  GO TO 8
    IQ = 88
    IF (DMU(I) .GE. .9E+12)  GO TO 8
    DO 7  K = 1,IS
    IF (K .EQ. J)  GO TO 7
    IQ = K
    IF (VNU(I,K) .NE. 0.)  GO TO 8
  7 CONTINUE
    VA = VNT(II)
    VNT(II) = VNT(I)
    VNT(I) = VA
    IOJ(J) = I
    LL(I) = 0
    LL(II) = 9
    GO TO 9
  8 CONTINUE
  9 CONTINUE
 99 RETURN
    END
```

```
      SUBROUTINE GIBBS(TE)
COMMENT.   COMPUTES INDIVIDUAL ENTHALPIES, ENTROPIES AND GIBBS FREE ENERGIES.
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), GA,
     1TAU, H(200), S0(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
    1 FORMAT(3HOT=F6.0,20H   H,S-D,MU-D, 3/LINE)
    2 FORMAT(3(1P3E12.4,I3,1H ) )
    3 FORMAT (10HODELETION A6, F10.4)
      THETA=TE/1000.
      DO 18 I=1,N
      TU1=TU(I,1)-10.
      TU2=TU(I,1)+10.
      TEQ=ABS(TU(I,1)-TL(I,2))
      Q=0.
      IF(TE.GE.TL(I,1).AND.TE.LE.TU(I,1)) GO TO 30
      IF(TE.GT.TL(I,2).AND.TE.LE.TU(I,2)) GO TO 31
      IF (TE .LE. 298.16) GO TO 30
      Q=1000000000000.
   31 K=2
      Y2=RA(I,K)+RB(I,K)*THETA+RC(I,K)*THETA**2+RD(I,K)*THETA**3
     1   +RE(I,K)*THETA**(-2)
      H2=(RF(I,K)+RA(I,K)*THETA+.5*RB(I,K)*THETA**2+(1./3.)*RC(I,K)
     1  *THETA**3+.25*RD(I,K)*THETA**4-RE(I,K)*1./THETA)*1000.
      SD2=CH(I,K)+RA(I,K)*ALOG(THETA)+RB(I,K)*THETA+.5*RC(I,K)*
     1   THETA**2+(1./3.)*RD(I,K)*THETA**3-.5*RE(I,K)*THETA**(-2)
      IF(TE.GE.TU1.AND.TE.LE.TU2.AND.TEQ.LE.1.) GO TO 32
      Y(I)=Y2
      H(I)=H2
      SD(I)=SD2
      GO TO 20
   32 K = 1
      Y1=RA(I,K)+RB(I,K)*THETA+RC(I,K)*THETA**2+RD(I,K)*THETA**3
     1   +RE(I,K)*THETA**(-2)
      H1=(RF(I,K)+RA(I,K)*THETA+.5*RB(I,K)*THETA**2+(1./3.)*RC(I,K)
     1  *THETA**3+.25*RD(I,K)*THETA**4-RE(I,K)*1./THETA)*1000.
      SD1=CH(I,K)+RA(I,K)*ALOG(THETA)+RB(I,K)*THETA+.5*RC(I,K)*
     1   THETA**2+(1./3.)*RD(I,K)*THETA**3-.5*RE(I,K)*THETA**(-2)
      GO TO 33
   30 K = 1
      Y1=RA(I,K)+RB(I,K)*THETA+RC(I,K)*THETA**2+RD(I,K)*THETA**3
     1   +RE(I,K)*THETA**(-2)
      H1=(RF(I,K)+RA(I,K)*THETA+.5*RB(I,K)*THETA**2+(1./3.)*RC(I,K)
     1  *THETA**3+.25*RD(I,K)*THETA**4-RE(I,K)*1./THETA)*1000.
      SD1=CH(I,K)+RA(I,K)*ALOG(THETA)+RB(I,K)*THETA+.5*RC(I,K)*
     1   THETA**2+(1./3.)*RD(I,K)*THETA**3-.5*RE(I,K)*THETA**(-2)
      IF(TE.GE.TU1.AND.TE.LE.TU2.AND.TEQ.LE.1.) GO TO 34
      Y(I)=Y1
      H(I)=H1
      SD(I)=SD1
      GO TO 20
   34 Y2=RA(I,K)+RB(I,K)*THETA+RC(I,K)*THETA**2+RD(I,K)*THETA**3
     1   +RE(I,K)*THETA**(-2)
      H2=(RF(I,K)+RA(I,K)*THETA+.5*RB(I,K)*THETA**2+(1./3.)*RC(I,K)
     1  *THETA**3+.25*RD(I,K)*THETA**4-RE(I,K)*1./THETA)*1000.
      SD2=CH(I,K)+RA(I,K)*ALOG(THETA)+RB(I,K)*THETA+.5*RC(I,K)*
     1   THETA**2+(1./3.)*RD(I,K)*THETA**3-.5*RE(I,K)*THETA**(-2)
   33 F2=-(TU(I,1)-10.-TE)/20.
      F1=1.-F2
      Y(I)=F1*Y1+F2*Y2
      H(I)=F1*H1+F2*H2
      SD(I)=F1*SD1+F2*SD2
```

```
   20 IF (Y(I) .GE. 0.)  GO TO 1888
      Q = 100000000000.
 1888 IF (W1(3) .LT. 0.)  Q = 0.
      IF (TE .LT. 298.16) H(I)=H(I) -(298.16-TE)*Y(I)
      IF (TE .LT. 298.16) SD(I)=SD(I)- Y(I)*ALOG(298.16/TE)
   18 DMU(I) = H(I) - TE*SD(I) + Q
      IF (KR(11) - 1)  21,19,21
   19 WRITE (6,1)TE
      WRITE (6,2)(H(I),SD(I),DMU(I),I, I=1,N)
   21 RETURN
      END
```

```
      SUBROUTINE GUESS(TE,P2)
COMMENT.   THIS ROUTINE COMES UP WITH A CRUDE COMPOSITION GUESS BUT IT S
C    TO GET CALCULATIONS OFF TO A FASTER START.
     1COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, ELOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(12), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     3,FLOOR
     1COMMON /IRPIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), PA(200,2), BB(200,2), PC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     4,LL(200)
      FLOOR=W27/10.**(6+KR(5))
   97 DO 89  J = 1,N
      VA = 0.0
      DO 88  I = 1,IS
   88 VA = VA + SQRT(ABS(C(I,J)))
   89 W3(J) = 10.0-VA
      CALL SLITE (1)
      CALL GIBBS (TE)
      DO 14  I = 1,N
   14 VNT(I) = 0.0
      CALL DEFIOJ
  771 CALL REACT(TE)
      DO 1  I = 1,N
    1 VLNK(I) = -VLNK(I)
      CALL RANK(IR,VLNK,N)
      DO 7  I = 1,N
      J = IR(I,1)
      IF (LL(J) .LE. 0)  GO TO 7
      IF (DMU(J) .GE. .9E+12)  GO TO 3
    2 CALL SETUP(Y,XMIN,XMAX,J)
      XMIN = .80*XMAX
    6 VNT(J) = XMIN + VNT(J)
      DO 4  L = 1,IS
      K = IOJ(L)
      IF (K .EQ. 0)  GO TO 4
      VNT(K) = VNT(K) - VNU(J,L)*XMIN
    4 CONTINUE
    3 CONTINUE
    5 CALL SLITE (0)
      CALL SLITE (1)
      DO 7  I = 1,N
    7 W3(I) = VNT(I)
   27 RETURN
      END
```

```
      SUBROUTINE H BAL (TE,PR, ENTR, LL)
COMMENT.   THIS ROUTINE COMPUTES A PRESSURE ENTHALPY POINT.
C  INPUT ENTHALPY IS W1(4) IN COMMON. IX WORKS THE SAME AS FOR EQUIL (WHICH SEE)
C     A VOLUME INPUT INSTEAD OF PRESSUR WORKS THE SAME WAY AS FOR EQUIL ALSO.
      COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), GH(10), RHO(10),
     2ISERI(10), WATE(20), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), GA,
     1TAU, H(200), SU(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W46, CP, EN, C(12,200), SPECIE(200)
      COMMON/SCRATC /HN(200,2)
  230 FORMAT (21HRESULTS NO DAMN GOOD )
      FTU = 6000.0
      FTL=75.
   55 CALL EQUIL (TE,PR,HE,ENTR,LL)
      LIM = 20
      DO 11  I = 1,LIM
      CALL SLITET(2,KOUNFX)
       GO TO(211,200),KOUNFX
  200 IF (HE - W1(4))  201,14,202
  201 FTL = TE
      FLP = VNT(NP)
      HLP = HE
      DO 70  L = 1,N
   70 HN(L,1) = VNT(L)
      GO TO 111
  202 FTU = TE
      FUP = VNT(NP)
      HUP = HE
      DO 71  L = 1,N
   71 HN(L,2) = VNT(L)
  111 K = 1
      CF= AMAX1(1.0,CF)
      CF = AMIN1(16.0, CF)
      DT = (W1(4) - HE)/(CF*CP)
      DT= AMIN1(DT, .5*(FTU-TE))
      DT= AMAX1(DT, .5*(FTL-TE))
      TE = TE + DT
      HOLD = HE
      IF (FTU-FTL .LT. 1.)  GO TO 21
      IF (ABS(DT) .LT. .1)  GO TO 14
      CALL EQUIL (TE,PR,HE,ENTR,LL)
   15 CF = (HE - HOLD)/(CP*DT)
   13 WRITE (6,230)
      WRITE (16,230)
   21 VA = (HUP-W1(4))/(HUP-HLP)
      VB = (W1(4)-HLP)/(HUP-HLP)
      CP = 0.
      DO 22  L = 1,N
      CP = CP + VNT(L)*Y(L)
      IF (LL .NE. 1)  GO TO 14
   22 VNT(L) = VA*HN(L,1) + VB*HN(L,2)
   14 ENTR = ENTR + (W1(4) - HE)/TE
      RETURN
      END
```

```
      FUNCTION IPHASE(L)
COMMENT       THIS ROUTINE DETERMINES WHAT CONDENSED PHASES ARE PRESENT.
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     3,FLOOR
      IPHASE = 0
      IF (IG .EQ. N)  GO TO 99
      INC = 1
      IGP = IG+1
      DO 12  I = IGP,N
      IF (VNT(I) .LE. FLOOR)  GO TO 12
      IPHASE = IPHASE + INC
   12 INC = INC + INC
   99 RETURN
      END




      SUBROUTINE LINDEP (I)
COMMENT. THIS ROUTINE ESTABLISHES LINEAR DEPENDENCE BY THE GRAM SCHMIDT-
C    TION AND THEN INVERTS THE A MATRIX BY THE METHOD OF CONJUGATE GRADIE
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      DIMENSION SS(12), D(12,12)
      D(I,I) = 1.
      IF (I .GT. IS)  GO TO 887
      IF (I .EQ. 1)  GO TO 8
      IM = I -1
      DO 7  J = 1,IM
      D(J,I) = 0.
      R = 0.0
      DO 2  K = 1,IS
      IF (A(K,I) .EQ. 0.)  GO TO 2
      IF (A(K,J) .EQ. 0.)  GO TO 2
      R = R + A(K,J)*A(K,I)
    2 CONTINUE
      IF (R .EQ. 0.)  GO TO 7
      Q = R/SS(J)
      VA = 0.
      DO 3  K = 1,IS
      A(K,I) = A(K,I) - Q*A(K,J)
      IF (A(K,I) .EQ. 0.)  GO TO 3
      VA = VA + ABS(A(K,I))
    3 CONTINUE
      IF (VA .LT. .1)  GO TO 6
      DO 17  K = 1,J
   17 D(K,I) = D(K,I) - Q*D(K,J)
    7 CONTINUE
    8 SS(I) = 0.
      DO 4  J = 1,IS
    4 SS(I) = SS(I) + A(J,I)**2
    5 CALL SLITE (2)
      IF (I .LT. IS)  GO TO 6
  887 DO 13  J = 1,IS
      DO 13  K = 1,IS
      VA = 0.
      DO 12  L = J,IS
   12 VA = VA + D(J,L)*A(K,L)/SS(L)
   13 A(K,J) = VA
  871 FORMAT (7F18.6)
    6 RETURN
      END
```

```
      SUBROUTINE ONE D (HSTAG,TZ,PZ,HZ,VZ,TO,PO,HO,VO,PS,AS,GT,GC,GV,LL)
COMMENT    CONTINUITY EQUATION FOR 1 DIMENSIONAL FLOW FOR ADIABATIC (19)
C     OR ISOTHERMAL (20) MODELS.
      COMMON A(12,12),KR(20)
      IF (KR(11) .NE. 0) WRITE (6,1122)PZ,PO
      IF (KR(11) .NE. 0) WRITE (6,1128) HZ,HO
 1128 FORMAT (' HX,HO'2E14.4)
      IF (KR(11) .NE. 0) WRITE (6,1124)TZ,TO
 1124 FORMAT(' TZ,TO'2E14.4)
      IF (KR(11) .NE. 0) WRITE (6,1123)VZ,VO
 1122 FORMAT (' PX,PO'2E14.4)
 1123 FORMAT(' VZ,VO'2E14.4)
      GT = ALOG(TO/TZ)/ALOG(PZ/PO)
      GV = ALOG(PO/PZ)/ALOG(VZ/VO)
      IF (KR(11) .NE. 0) WRITE (6,1125)GV,GT
 1125 FORMAT (' GV,GT'2E14.4)
      LL = 1
      IF (ABS(TZ-TO) .GT. 3.)  GO TO 19
      LL = 2
      GC = (HO-HZ)/ALOG(PO/PZ)
      IF (KR(11) .NE. 0) WRITE (6,1127) GC,HSTAG
 1127 FORMAT (' GC,HSTAG'2E14.4)
      PSTAR = PZ*EXP(-GV/2. + (HSTAG-HZ)/GC)
      HSTAR = HZ + GC*ALOG(PSTAR/PZ)
      IF (KR(11) .NE. 0) WRITE (6,1129)PSTAR,HSTAR
 1129 FORMAT (' PSTAR,HSTAR' 2E14.4)
      VSTAR = VZ*(PZ/PSTAR)**(1./GV)
      GO TO 20
   19 GC = (HO-HZ)/(PO*VO - PZ*VZ)
      PSTAG = PZ*(1. +(HSTAG - HZ)/GC/PZ/VZ)**(GV/(GV-1.))
      PSTAR = PSTAG*(2./(GV+1.))**(GV/(GV-1.))
      VSTAR = VZ*(PZ/PSTAR)**(1./GV)
      HSTAR = HZ + GC*(PSTAR*VSTAR - PZ*VZ)
   20 AS = VSTAR/SQRT(HSTAG-HSTAR)
      PS = PSTAR
      RETURN
      END
```

```
      SUBROUTINE OUT (PR,TE,HE,ENTR,NS)
COMMENT.   COMPOSITION AND STATE VARIABLE OUTPUT ROUTINE.
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     3,FLOOR
     0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), GA,
     1TAU, H(200), SU(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      DIMENSION SPOT(4), VOT(4)
  102 FORMAT (/'  T(K)   T(F)   P(ATM)    P(PSI) ENTHALPY  ENTROPY   CP/CV
     X    GAS    RT/V')
  104 FORMAT (2F6.0,F8.2,F9.2,F9.2,F9.2,F8.4,F7.3,F8.3)
   44 FORMAT (4(1X,F9.5,1X,A6))
   45 FORMAT(4(1X,1PE9.2,1X,A6))
   21 FORMAT (1H )
      GAMMA = CP/(CP - 1.9871*FN)
      TF = 1.8*TE - 459.4
      VH = HE/1000.0
      PF = PR*14.70069
      WRITE (6,102)
```

```
   13 WRITE(6,104) TE,TF,PR,PF,VH,ENTR,GAMMA,FN,VNT(NP)
      WRITE (6,21)
      CALL RANK(IR, VNT, N)
      J = 1
      DO 904 II= 1,N
      I = IR(II,1)
      IF (VNT(I) .LE. FLOOR)  GO TO 904
      SPOT(J) = SPECIE(I)
      VOT(J) = VNT(I)
      J = J + 1
      IF (J .LT. 5)  GO TO 904
      IF (VOT(1) .GT. .009995)  WRITE (6,44)(VOT(K),SPOT(K),K=1,4)
      IF(VOT(1) .LE. .009995)  WRITE(6,45)(VOT(K),SPOT(K),K=1,4)
      J = 1
  904 CONTINUE
      J = J -1
      IF (J .NE. 0) WRITE (6,45)(VOT(K),SPOT(K),K=1,J)
  170 RETURN
      END
```

```
COMMENT.   THIS PROGRAM CONSISTS OF ROUTINES PEP, TSALT, DESNOZ, BOOST, TSBAL,
C      TABLO, TWID, SLTUP, REACT, ADJUST, RANK, OUT,STOICH, EQUIL, PUTIN,
C      DEFIOJ, CNED, IPHASE, THERMO, GIBBS, TWITCH,          HBAL, DESIGN, SEARCH,
C    LINDEP, SBAL, GUESS, TAPEB AND FIXBAS)
COMMENT.   THE MAIN PROGRAM CONTROLS THE INPUT AND OUTPUT AND ESTABLISHES THE
C    PROPELLANT THERMODYNAMIC MODEL IN THE WAY IT CALLS HBAL AND SBAL.
      0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
      1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
      2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      3,FLOOR
      0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
      1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DNU(200), VLNK(200),
      210J(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
      3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      4,LL(200)
       COMMON/MOON/TSTEST,TE,IRUN
       CALL SETCLK
       IRUN = 0
       TCH = 3000.
     8 TE= AMAX1(TCH, 500.0)
       TSTEST = 0.
       TE = AMIN1(TE,5000.)
       CALL PUT IN (LE)
C  THE NEXT STATEMENT DELETES CALCULATION WHEN INPUT ERRORS ARE FOUND.
       IF (LE .EQ. 1)  STOP
       PR = W1(5)
       IF (KR(19) .EQ. 1)  GO TO 15
       CALL GUESS (TE,PR)
   15 IF (KR(7) .EQ. 0)  GO TO 14
       TE = W1(6)
       VNT(NP) = ALOG(.08205*W1(6)/W1(5))
       CALL EQUIL (TE, PR, HE, SE, 1)
       PR = FN*VNT(NP)
       SYSENT = SE
       GO TO 114
   14 CALL H BAL (TE, PR, SYSENT, 1)
   12 TCH = TE
       HE = W1(4)
       CHN = FN
```

```
  114 CALL OUT (PR,TE,HE,SYSENT,1)
      IF (KR(1) .EQ. 1)  GO TO 8
      IF (W1(5) .GE. W1(6))  GO TO  125
      WRITE ( 6,3)
    3 FORMAT (/' WHY IS THE EXIT PRESSURE .GE. THE CHAMBER PRESSURE.')
      GO TO 8
  125 CALL DESIGN (TE, PR, HE, SYSENT, 0, 1)
      PR = W1(6)
      CALL S BAL (TE, PR, HE, SYSENT, TCH, 0)
      CALL DESIGN (TE, PR, HE, SYSENT, 0, 2)
   22 TE = .5*(TCH+TE)
   70 CALL S BAL (TE, PP, HE, SYSENT, TCH, 1)
      CALL OUT (PR,TE,HE,SYSENT,2)
      FLOOR=W27*1.E-7
      CALL DESIGN (TE, PR, HE, SYSENT, 1, 2)
      IF (KR(3) .EQ. 0)  CALL DESNOZ
      GO TO 8
      END



      SUBROUTINE PUT IN (LE)
COMMENT     INPUT ROUTINE CALLED BY MAIN PROGRAM.
CALLS ROUTINES DATE & TOFDAY (TIME OF DAY) WHICH MAY BE DELETED
C ALSO NOTE DELETABLE ROUTINES SETCLK AND LKCLKS THAT MEASURE CPU TIME
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     3,FLOOR,ITAG(100),WING(10)
      COMMON/MOON/TSTEST,TE,IRUN
      DIMENSION JE(10,6), JIE(10,6),SWING(10)
      DIMENSION ATWT(100)
      DATA (ATWT(I), I = 1,100)/1.008, 4.003, 6.94, 9.013, 10.82, 12.011
     1,14.008, 16., 19., 20.183, 22.991, 24.32, 26.98, 28.09, 30.975,
     2 32.066, 35.457, 39.944, 39.1, 40.08, 44.96, 47.9, 50.95, 52.01,
     4 54.94, 55.85, 58.94, 58.71, 63.54, 65.38, 69.72, 72.6, 74.92,
     5 78.96, 79.916, 83.80, 85.48, 87.63, 88.91, 91.22, 92.91, 95.95,
     6 99., 101.1, 102.91, 106.4, 107.88, 112.41, 114.82, 118.7, 121.76,
     7 127.61, 126.91, 131.3, 132.91, 137.36, 138.92, 140.13, 140.91,
     8 144.27, 147., 150.35, 152., 157.26, 158.93, 162.51, 164.94, 167.2
     97, 168.94, 173.04, 174.99, 178.50, 180.95, 183.86, 186.22, 190.2,
     1 192.2, 195.09, 197., 220.61, 204.39, 207.21, 208.99, 210., 210.,
     2 222., 223., 226., 227., 232., 231., 238., 237., 237.,12.01,9.031,
     310.82,24.32,26.98, 253. /
    1 FORMAT (19I1, A1, A6, I4, 5X, I5)
    2 FORMAT (5A6, 6(I3, A2), F7.0, F6.0)
222   FORMAT(5A6,6(I3,A2),F5.0,F6.0)
82    FORMAT(1X,5A6,6(I3,A2), F5.0, F6.0)
    3 FORMAT (12F6.6, A6, A2)
      CALL LKCLKS(VB)
      CALL SETCLK
      WRITE(6,8889)VB
8889  FORMAT('0(CPU'F6.2,'SECS.)')
      LE = 0
      IF (IRUN)  19,11,19
   11 WRITE (6,1200)
 1200 FORMAT('1 1978 VERSION OF PEP.')
7771  WRITE(6,1120)
 1120 FORMAT (/'0PUTIN OPTS, NAME, NO.OF INGRDS.(M), + NO.OF RUNS(N)')
      WRITE (6,1129)
 1129 FORMAT ('0 1234567890          (NAME)   M          N')
      READ (5,1)(KR(I),I =1,19),ISERI(1),ISERI(2),IN,I
     XRUN
      DO 12  I = 1,12
   12 JAT(I) = 0
      IF (KR(9) .NE. 0)  WRITE (6,1121)
```

```
 1121 FORMAT ('0NOW READ IN INGREDIENT SERIAL NUMBERS ENDING UNDER V.'/'
     X     V     V     V     V     V     V     V     V     V')
       IF (KP(9) .NE. 0)  READ (5,1112) (ITAG(I),I=1,IN)
       IF(KP(9) .NE. 0) WRITE(6,1112)(ITAG(I),I=1,IN)
 1112 FORMAT (10I5)
       KP=1
       REWIND 11
       READ(11,1110)VA
       DO 13  I = 1,IN
 1110 FORMAT (11A6,A5)
 1111 FORMAT(' '11A6,A5)
       IF (KP(9) .EQ. 0)  GO TO 1114
       K=ITAG(I)
       IF (KP .LT. K)  GO TO 1117
       REWIND 11
       READ(11,1110)VA
       KP=1
 1117 DO 1113 J=KP,K
       IF(J .NE. K)READ(11,2)
       IF(J .NE. K) GO TO 1113
       READ (11,222)(BLOK(I,L),L=1,5),(JIE(I,L),JE(I,L),L=1,6)
      *,DH(I),RHO(I)
 1113  CONTINUE
       KP=K+1
       GO TO 1115
 1114 READ ( 5,2)(BLOK(I,J),J=1,5),(JIE(I,J),JE(I,J),J=1,6)
      *,DH(I),RHO(I)
 1116 FORMAT (10A6,2X,A6,A5)
 1115 DO 13 J=1,5
       IE(I,J)=JE(I,J)
   13 FIE(I,J)=JIE(I,J)
       IF (KP(10) .EQ. 0) GO TO 1201
       WRITE(6,1205),IN
 1205 FORMAT('0TO CHANGE DH & RHO, TYPE COUNT(1-'I2'), DH &RHO.'/
      &'     V          V          V')
       DO 1204 J=1,IN
       READ(5,1203)I,VA,VB
 1203 FORMAT(I5,2F10.0)
       IF(I .EQ. 0)GO TO 1201
       DH(I)=VA
 1204 RHO(I)=VB
 1201 CONTINUE
       CALL STOICH(LE)
       DO 14  I = 1,IN
       WATE(I) = 0.
       DO 14  J = 1,IS
       K = JAT(J)
   14 WATE(I) = WATE(I) + AMAT(I,J)*ATWT(K)
       CALL SEARCH(LE)
   19 CONTINUE
   18 WRITE (6,1122)
 1122 FORMAT ('0READ IN CH. P, EX. P, WT1, WT2, + ETC.'/' (TO READ NEW C
      XONTROL CARD HIT CAR. RET.)')
       WRITE (6,1123)
 1123 FORMAT ('      V     V     V     V     V     V     V     V     V')
       READ (5,3) W1(5), W1(6), (WING(I), I = 1,10),ISERI(3), ISERI(4)
       IF (W1(5) .EQ. 0.)  GO TO 7771
       IF (KP(2) .NE. 1)  GO TO 20
       IS = IS -1
   20 IRUN = IRUN - 1
       KP(19) = 1
       IF (WING(1) .EQ. 0.)  GO TO 120
       KP(19) = 0
       DO 21  J = 1,IS
       ALP(J) = 0.
       DO 21  I = 1,IN
```

```
   21 ALP(J) = ALP(J) + AMAT(I,J)*WING(I)/WATE(I)
      W27 = 0.
      W1(4) = 0.
      W43 = 0.
      VA = 1.
      DO 22  I = 1,IN
      SWING(I) = WING(I)
      W1(4) = W1(4) + DH(I)*WING(I)
      W27 = W27 + WING(I)
      IF (RHO(I))  25,25,24
   24 W43 = W43 + WING(I)/RHO(I)
      GO TO 22
   25 VA = 0.
   22 CONTINUE
      W43 = VA/W43  *W27
  120 IF (KR(4) .NE. 1)  GO TO 23
      IF (KP(17) .EQ. 1)  GO TO 23
      W1(5) = W1(5)/14.70069
      IF (KR(7) .EQ. 1)  GO TO 23
      W1(6) = W1(6)/14.70069
      CALL DATE(ISERI(3))
      CALL TOFDAY(ISERI(5))
   23 WRITE (6,16) (ISERI(I), I = 2,6)
   16 FORMAT('1',5A6,6X,'DH   COMPOSITION'/)
      DO 27  I = 1,IN
      DO 135 L=1,6
      IF(JIE(I,L) .EQ. 0) GO TO 136
  135 CONTINUE
  136 L=L-1
      IDH=DH(I)
   27 WRITE(6,83)(BLOK(I,J),J=1,5),IDH,(JIE(I,J),JE(I,J),J=1,L)
   83 FORMAT(2X, 5A6, I7,2X,6(I2,A2))
      WRITE (6,5575)(SWING(II),II=1,IN),W27
 5575 FORMAT('1INGRED.WTS.&TOTAL/ GRAM ATOMS/ CHAMBER/ EXHAUST RESULTS/
     *PERFORMANCE'//(7F10.5))
      WRITE (6,301)(ALP(I),ASPEC(I),I=1,IS)
  301 FORMAT (/5(F10.6,1X,A2,1X))
      IF (KR(2) .NE. 1)  GO TO 28
      IS = IS + 1
   28 IF (LE .NE. 1)  GO TO 29
      IF (IRUN .EQ. 0)  GO TO 29
      DO 30  I = 1,IRUN
   30 READ (5,1)
      WRITE ( 6,33)
      IRUN = 0
   33 FORMAT(/' AT THIS POINT THE PROGRAM WILL ATTEMPT THE NEXT RUN.')
   29 RETURN
      END


      SUBROUTINE RANK(IR,Y,N)
COMMENT.  RANKS VECTOR Y IN DESCENDING ORDER, RANKINGS APPEAR IN IR(I,1).
      DIMENSION X(200), Y(200), IR(200,2)
      DO 1  I = 1,N
      IR(I,2) = IR(I,1)
    1 X(I) = AMAX1(Y(I), .0)
      DO 4  I = 1,N
      S = -1.0
      DO 3  J = 1,N
      IF (S - X(J)) 2,3,3
    2 IR(I,1) = J
      S = X(J)
    3 CONTINUE
      J = IR(I,1)
    4 X(J) = -1.0
      RETURN
      END
```

```
      SUBROUTINE REACT(TE)
COMMENT, THIS ROUTINE COMPUTES THE STOICHIOMETRIC COEFFICIENTS AND LOG EQUILIBRI
C    UM CONSTANTS FOR ALL REACTIONS IN TERMS OF THE CURRENT BASIS.
      OCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
      1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
      2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      OCOMMON /1BRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
      1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
      2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
      3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
       CALL SLITET(1,KOUOFX)
        GO TO(21,31),KOUOFX
   21 DO 11 K = 1,IS
      DO 11 J = 1,N
      VNU(J,K) = 0.0
      DO 1  I = 1,IS
    1 VNU(J,K) = VNU(J,K) + A(I,K)*C(I,J)
      IF (ABS(VNU(J,K)) - .0051)  10,10,11
   10 VNU(J,K) = 0.0
   11 CONTINUE
   31 VA = 1./1.9871/TE
      DO 3  I = 1,N
      VB = 0.0
      DO 2  LS = 1,IS
      IF (VNU(I,LS)) 17,2,17
   17 J = IOJ(LS)
      VB = VB + VNU(I,LS)*DMU(J)
    2 CONTINUE
      VLNK(I) = VA*(DMU(I) - VB)
    3 CONTINUE
      IF (KP(14) -1)  7,4,7
    4 WRITE (6,5)
      WRITE (6,6)(VLNK(I), I = 1,N)
      WRITE (6,8)(IOJ(I), I = 1,IS)
    8 FORMAT (10(5X,I7))
    5 FORMAT (22HOLOGS OF EQUIL CONST,S)
    6 FORMAT (1H 1PE11.4, 9E12.4)
    7 RETURN
      END



      SUBROUTINE S BAL (TE, PR, HE, SYSENT, TCH, LL)
      OCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
      1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
      2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      OCOMMON /1BRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
      1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
      2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
      3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      COMMON/SCRATC /HN(200,2)
  236 FORMAT (21HORESULTS NO DAMN GOOD )
      DIMENSION FAC(2)
      FTU = TCH
      FTL=75.
      LIM = 20
   88 CALL EQUIL(TE,PR,HE,ENTR,LL)
   89 CF = FAC(LL+1)
      DO 15  J = 1,LIM
      CALL SLITET(3,KOOOFX)
       GO TO(4115,210),KOOOFX
  210 IF (ENTR - SYSENT)  211,18,212
  211 FTL = TE
      FLP = VNT(NP)
      SLP = ENTR
      DO 70  L = 1,N
```

```
   70 HN(L,1) = VNT(L)
      GO TO 4115
  212 FTU = TE
      FUP = VNT(NP)
      SUP = ENTR
      DO 71  L = 1,N
   71 HN(L,2) = VNT(L)
 4115 CF= AMAX1(1.0,CF)
      CF = AMIN1(16.0, CF)
      VO = (SYSENT - ENTR)/CP/CF
      DT = TE*VO
      IF (VO)  131,133,133
  131 DT = TE*(EXP(VO) - 1.0)
  133 DT= AMIN1(DT, .5*(FTU-TE))
      DT= AMAX1(DT, .5*(FTL-TE))
  137 TE = TE + DT
      HENT = ENTR
      IF (FTU-FTL .LT. 2.)  GO TO 21
      IF (ABS(SYSENT-ENTR)/SYSENT .LT. .0001)  GO TO 18
      CALL EQUIL (TE,PR,HE,ENTR,LL)
   15 CF= ((ENTR-HENT)/(CP*ALOG(TE/(TE-DT))))
   17 WRITE (6,236)
   21 VA = (SUP-SYSENT)/(SUP-SLP)
      VB = (SYSENT-SLP)/(SUP-SLP)
      CP = 0.
      DO 22  L = 1,N
      CP = CP + VNT(L)*Y(L)
      IF (LL .NE. 1)  GO TO 18
   22 VNT(L) = VA*HN(L,1) + VB*HN(L,2)
   18 HE = HE + TE*(SYSENT - ENTR)
      FAC(LL+1) = CF
      RETURN
      END
```

```
      SUBROUTINE SEARCH(LE)
C . . . . TAPE SEARCH ROUTINE FOR THERMO DATA.
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATL(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), GA,
     1TAU, H(200), S0(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      INTEGER S
    1 FORMAT (1H A6, I6)
    4 FORMAT (34HO MARK. NO COMBUSTION SPECIES FOR A6,14H REVISE PEPAUX)
      IF (KR(2) .NE. 1)  GO TO 10
      IS = IS + 1
      JAT(IS) = 0
      ALP(IS) = 0.
   10 NP = 1
      CALL TAPEB (1,0,0,0)
      DO 99  LIM = 1,7777
      DO 9  I = 1,IS
    9 C(I,NP) = 0.
      CALL TAPEB (2,NP, KHASE, S)
      IF (KHASE .LT. 0)  GO TO 100
C . . . . SEE IF SPECIES BELONGS TO ELEMENT GROUP.
      IF (IE(1,1) .EQ. 0)  GO TO 99
   15 DO 18  I = 1,7
      IF (IE(I,1))16,19,16
```

```
   16 DO 17  J = 1,IS
      IF (IE(I,2) .NE. JAT(J))  GO TO 17
      C(J,NP) = IE(I,1)
      GO TO 18
   17 CONTINUE
      GO TO 99
   18 CONTINUE
   19 CONTINUE
   23 NP = NP +1
      IF (KHASE .NE. 1)  GO TO 98
      IG = NP -1
   98 IF (NP .LT. 200)   GO TO 99
      WRITE (6,5)
    5 FORMAT (51HONO. OF COMBUS. SPECIES EXCEEDS PROG. LIMIT OF 200  )
99    CONTINUE
  100 N = NP -1
      REWIND 12
      DO 50  I = 1,N
      W3(I) = 50.
      DO 50  J = 1,IS
   50 W3(I) = W3(I) - SORT(ABS(C(J,I)))
      DO 51  J = 1,IS
      H(J) = 0.
      DO 51  I = 1,N
   51 H(J) = H(J) + ABS(C(J,I))
      DO 53  J = 1,IS
      IF (H(J))  52,52,53
   52 WRITE ( 6,4) ASPEC(J)
      LE = 1
   53 CONTINUE
      IF (KR(8) .NE. 0) WRITE (6,1124)(SPECIE(I),I=1,N)
 1124 FORMAT ('0COMPLETE SPECIES LIST FOLLOWS'/(1X,11A6))
      RETURN
      END
```

```
      SUBROUTINE SETUP(X,XMIN,XMAX, J)
COMMENT.    THIS ROUTINE DETERMINES THE MAXIMUM AND THE MINIMUM CHANGE
C    ALLOWABLE IN REACTION COORDINATE J BEFORE NEGATIVE CONCENTRATIONS ARISE.
C    IT ALSO SETS UP THE FUGACITY COEFFICIENTS FOR REACTION J IN X(J).
      DIMENSION X(30)
      COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2)SERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SO(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      XMAX = .100000000E+16
      XMIN =-.100000000E+16
      DO 9  I = 1,IS
      X(I) = 0.
      IF (VNU(J,I) .EQ. 0.)  GO TO 9
      K = IOJ(I)
      VO = VNT(K)
      IF (IG .LT. K)  GO TO 6
    4 X(I) = VNU(J,I)
    5 IF(VNU(J,I))  3,9,7
    7 XMAX= AMIN1(XMAX, VO/VNU(J,I))
      GO TO 9
    3 XMIN= AMAX1(XMIN, VO/VNU(J,I))
    9 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE SLITE(J)
      DIMENSION LIT(4)
      IF (J .EQ. 0) GO TO 9
      LIT(J)=1
      GO TO 99
9     DO 10 I=1,4
10    LIT(I)=0
      GO TO 99
      ENTRY SLITET(J,K)
      K=2
      IF (LIT(J) .EQ. 0) GO TO 99
      K=1
      LIT(J)=0
99    RETURN
      END
```

```
      SUBROUTINE STOICH(LE)
COMMENT PROPELLANT STOICHIOMETRY ROUTINE CALLED BY PUTIN.
COMMENT.    ALIASES.  U1= UNBURNED BERYLLIUM, U2 = UNBURNED BORON,
C       U3 = UNBURNED MAGNESIUM, U4 = UNBURNED ALUMINUM,
C     U5 = UNBURNED CARBON,   DON,T USE U6.      THESE INERTS MELT AND
C   EVAPORATE BUT DO NOT REACT.    GAS SPECIES MAY BE ELIMINATED FROM PERMIX
C      TAPE TO PREVENT EVAPORATION.
      COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2USER(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     3,FLOOR,ITAG(100),WING(10)
      DIMENSION SYMB(100)
      DIMENSION FE (10,6)
      EQUIVALENCE (FE(1,1), IE(1,1))
      DATA (SYMB(I), I = 1,100)/                                  600HH      HE
     1LI    BE     B      C      N      O      F      NE     NA     MG     AL
     2SI    P      S      CL     AP     K      CA     SC     TI     V      CR
     3MN    FE     CO     NI     CU     ZN     GA     GE     AS     SE     BR
     4KR    RB     SR     Y      ZR     NB     MO     TC     RU     RH     PD
     5AG    CD     IN     SN     SB     TE     I      XE     CS     BA     LA
     6CE    PR     ND     PM     SM     EU     GD     TB     DY     HO     ER
     7TM    YB     LU     HF     TA     W      RE     OS     IR     PT     AU
     8HG    TL     PB     BI     PO     AT     RN     FR     RA     AC     TH
     9PA    U      NP     U      U5     U1     U2     U3     U4     FM
    1 FORMAT (8HOWHAT,S A6)
    2 FORMAT (/' INGREDIENT CARD 'I2,' GOOFED UP.')
      DO 11  I = 1,100
   11 ITAG(I) = 0
      DO 19  I = 1,IN
      DO 18  J = 1,6
      IF (FIE(I,J))  14,19,12
   12 DO 17  L = 1,100
      IF (FE(I,J) - SYMB(L))  17,13,17
   13 ITAG(L) = 1
      IE(I,J) = L
      GO TO 18
   17 CONTINUE
      WRITE ( 6,1) IE(I,J)
    4 WRITE ( 6,2) I
      LE = 1
    8 CONTINUE
   19 CONTINUE
      IS = 1
      DO 25  I = 1,100
      IF (ITAG(I))  25,25,20
```

```
   20 ASPEC(IS) = SYMB(I)
      JAT(IS) = I
      IS = IS + 1
   25 CONTINUE
      IS = IS - 1
      DO 31  I = 1,IN
      DO 26  J = 1,12
   26 AMAT(I,J) = 0.
      DO 29  K = 1,IS
      DO 28  J = 1,6
      IF (IE(I,J) - JAT(K))  28,27,28
   27 AMAT(I,K) = FIE(I,J)
      GO TO 29
   28 CONTINUE
   29 CONTINUE
   31 CONTINUE
      RETURN
      END
```

```
      SUBROUTINE TABLO(II,JJ,KK)
COMMENT.   WHEN THE BASIS IS NO LONGER OPTIMUM, THIS ROUTINE CHANGES IT BY
C    THE TABLEAU METHOD OF LINEAR PROGRAMMING.
     DCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IC, NP, VNT(201), W47, NAME, SER
     DCOMMON /IRRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SU(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     4,LL(200)
      COMMON/MOON/TSTEST,TE
  104 DO 19  L = 1,N
      IF (LL(L) .LT. 0)  GO TO 19
      IF (L .EQ. JJ)  GO TO 19
      IF (ABS(VNU(L,KK)) .LT. .0001)  GO TO 19
      VA = -VNU(L,KK)/VNU(JJ,KK)
      DO 15  M = 1,IS
   15 VNU(L,M) = VNU(L,M) + VA*VNU(JJ,M)
      VNU(L,KK) = -VA
      DO 16  M = 1,IS
      IF (ABS(VNU(L,M)) .GT. .00001)  GO TO 16
      VNU(L,M) = 0.
   16 CONTINUE
   19 CONTINUE
      DO 20  M = 1,IS
   20 VNU(JJ,M) = 0.
      VNU(JJ,KK) = 1.
      IOJ(KK) = JJ
      LL(JJ) = 0
      LL(II) = 9
      CALL REACT(TE)
      IF (KR(15) .NE. 1)  GO TO 99
      WRITE (6,999)II,JJ,KK,SPECIE(II),SPECIE(JJ)
  999 FORMAT (3I5, 3X, A6, ' REPLACED BY ', A6)
   99 RETURN
      END
```

```
      SUBROUTINE TAPEB (IW, L, PHASE, S)
COMMENT.   THIS ROUTINE BUFFERS THE INPUT FROM THE LIBRARY TAPE.  THIS SPEEDS
C    INPUT ON THE UNIVAC BUT MAY SLOW IT ON A GOOD MACHINE.
      OCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
      1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
      2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      OCOMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
      1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DHU(200), VLNK(200),
      2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
      3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      DIMENSION BIN(20,35)
      GO TO (11,21), IW
   11 REWIND 12
      I = 20
      GO TO 99
   21 I = I + 1
      IF (I .LT. 21)  GO TO 31
      I = 1
      READ (12) ((BIN(J,K),K = 1,35),J=1,20)
   31 PHASE = BIN(I,1)
      SPECIE(L) = BIN(I,2)
      S = BIN(1,3)
      DO 41  J = 1,7
      K = 3 + 2*(J-1)
      IE(J,1) = BIN(I,K+1)
   41 IE(J,2) = BIN(I,K+2)
      RA(L,1) = BIN(I,18)
      RB(L,1) = BIN(I,19)
      RC(L,1) = BIN(I,20)
      RD(L,1) = BIN(I,21)
      RE(L,1) = BIN(I,22)
      RF(L,1) = BIN(I,23)
      CH(L,1) = BIN(I,24)
      TL(L,1) = BIN(I,25)
      TU(L,1) = BIN(I,26)
      RA(L,2) = BIN(I,27)
      RB(L,2) = BIN(I,28)
      RC(L,2) = BIN(I,29)
      RD(L,2) = BIN(I,30)
      RE(L,2) = BIN(I,31)
      RF(L,2) = BIN(I,32)
      CH(L,2) = BIN(I,33)
      TL(L,2) = BIN(I,34)
      TU(L,2) = BIN(I,35)
   99 RETURN
      END
```

```
      SUBROUTINE THERMO(TE,HE,ENTR)
COMMENT.   COMPUTES SYSTEM ENTHALPY, ENTROPY AND HEAT CAPACITY
      OCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
      1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
      2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      OCOMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
      1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DHU(200), VLNK(200),
      2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
      3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      VH = 0.0
      VS = 0.0
      CP = 0.0
      DO 11  I = 1,N
      CP = CP  + VNT(I)*Y(I)
      VH = VH  + VNT(I)*H(I)
```

```
   11 VS = VS  + VNT(I)*SD(I)
      FN = 0.0
      VSM = 0.C
      DO 12  I = 1,IG
      IF(VNT(I) .LE. 0.)GO TO 12
      FN = FN  + VNT(I)
      VSM= VSM+ VNT(I)*ALOG(VNT(I))
12    CONTINUE
      VSM = 1.9871*(VSM + FN*VNT(NP))
      HE = VH
      ENTR = VS - VSM
      RETURN
      END



      SUBROUTINE TSALT(TE,PR,HE,ENTR,PUPI,PLOI)
COMMENT.      THIS SUBROUTINE COMPUTES COMPOSITION, PRESSURE AND ENTHALPY
C     GIVEN TEMPERATURE AND ENTROPY. IT IS CALLED BY TSBAL.
      COMMON A (12,12),KR(20)
      COMMON/MOON/TSTEST
      TSTEST = -217.1936
      PLO = PLOI
      PUP = PUPI
      PR=(PUP+PLO)/2.
      DO 22  JI = 1,20
      CALL EQUIL(TE,PR,HE,SE,1)
      IF (KR(13) .NE. 0) WRITE(6,9)JI,TE,SE,PUP,PLO
    9 FORMAT (' TSBAL*I5,F8.1,3F12.3)
      IF (SE .GT. ENTR) PLO=PR
      IF (SE .LT. ENTR) PUP=PR
      PR=(PUP+PLO)/2.
  166 IF ((PUP-PLO)/PLO .LT. .00008)   GO TO 23
   22 CONTINUE
      WRITE (6,1)
    1 FORMAT (' TSALT STOP')
      CALL SLITE (3)
   23 TSTEST = 0.
      RETURN
      END



      SUBROUTINE TSBAL(TE,PR,HE,ENTR,PUPI,PLOI)
COMMENT.      THIS SUBROUTINE COMPUTES COMPOSITION, PRESSURE AND ENTHALPY
C     GIVEN TEMPERATURE AND ENTROPY.   IT IS CALLED BY TSBAL.
      DCOMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(30), RHO(10),
     2ISERI(10), MATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      DCOMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), PA(200,2), PB(200,2), PC(200,2), PD(200,2), PE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      DIMENSION X(12), XM(12)
    6 FORMAT (I5,F10.0, F12.3)
    9 FORMAT (1P 10E13.4)
      KR(18)=1
      PR=.5*(PUPI +PLOI)
  1734 CALL GIBBS(TE)
      CALL FIXBAS
   12 DO 38  J = 1,IS
      X(J) = 0.
      XM(J) = 0.
      DO 31  I = 1,N
      IF (C(I,J) .EQ. 0.)  GO TO 31
```

```
      XM(J) = AMAX1(VNT(I), XM(J))
      X(J) = X(J) + C(J,I)*VNT(I)
   31 CONTINUE
      IF (ABS(ALP(J) - X(J))/XM(J) .LT. .00001)  GO TO 36
      CALL SLITE(1)
      GO TO 39
   38 CONTINUE
   39 CALL DEFIOJ
      CALL REACT (TE)
      DO 211  I = 1,N
  211 W3(I) = 50.0 -VLNK(I)
      CALL RANK(IR,W3,N)
   11 DO 22  JC = 1,20
      PR=AMAX1(PLOI,PR)
      PR=AMIN1(PUPI,PR)
      CALL TWITCH(PR,0)
      CALL THERMO (TE,HE,STRY)
      VX=1.
      IF (JC .GT. 5) VX=2.
      IF (JC .GT. 10) VX=4.
      PR=PR*EXP(-(ENTR-STRY)/(FN*VX)/1.9871)
      CALL SLITET(4,KODEFX)
       GO TO(146,17),KODEFX
  146 IF (KR(13)-1)  15,14,15
   14 WRITE (6,8)JC,TE,PR
      WRITE (6,9)(VNT(I), I = 1,N)
   15 DO 23  ICC = 1,3
   25 CALL TWITCH(PR,1)
      CALL THERMO (TE,HE,STRY)
      PR=PR*EXP(-(ENTR-STRY)/(FN*VX)/1.9871)
      CALL SLITET(4,KODEFX)
       GO TO(23,22),KODEFX
   23 CONTINUE
   22 CONTINUE
      KR(18)=0
   18 CALL TSALT(TE,PR,HE,ENTR,PUPI,PLOI)
   17 VNT(NP) = EXP(VNT(NP))
      RETURN
      END
```

```
      FUNCTION TWID (X)
COMMENT.   COMPUTES THE EQUILIBRIUM FUNCTION.
      COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATER(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SO(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      DIMENSION X(30)
      VA = 0.0
      TWID = 0.0
      DO 1  I = 1,IS
      IF (X(I) .EQ. 0.)  GO TO 1
   11 VA = VA + X(I)
      K = IOJ(I)
      IF (VNT(K) .LE. 0.) GO TO 1
  111 TWID= TWID+ X(I)*ALOG(VNT(K))
    1 CONTINUE
      TWID = TWID + VA*VNT(NP)
      RETURN
      END
```

```
      SUBROUTINE TWITCH(PR,JG)
COMMENT.   THIS IS THE ROUTINE WHICH CONVERGES ON CHEMICAL COMPOSITION.
CALLED BY EQUIL.
     1COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1IFIE(10,6), IE(20,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     3,FLOOR
     1COMMON /EQBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), GA,
     1TAU, H(200), SG(200), Y(200), JC, IP(200,2), DMU(200), VLNK(200),
     2IOJ(10), PA(200,2), RR(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     4,LL(200)
      DIMENSION X(30)
      IC = 0
      VQQ = JC -1
      VQQ = .5 - VQQ/20.
      VQQ = AMAX1(.05, VQQ)
      VC = 0.0
      IF  (KR(17) - 1)   401,402,401
  401 DO 200  I = 1,IG
  200 VC = VC + VNT(I)
      VNT(NP) = ALOG(PR/VC)
  402 DO 99  J = 1,N
      IF (LL(J) .LE. 0)  GO TO 99
      IF (JG .NE. 0  .AND.  LL(J) .NE. 9)  GO TO 99
      KICK = 0
      VC = VQQ
    7 CALL SETUP (X, XMIN, XMAX, J)
      IF (VNT(J) .GT. 0.)  GO TO 22
      DX = - 1.001*VNT(J) + FLOOR
      GO TO 97
   22 CONTINUE
      VA = VLNK(J) - TWIN (X)
      VB = 0.0
      LL(J) = 1
      IF (J.LE.IG)  GO TO 4
COMMENT       MAJOR SPECIES TOLERANCE
    3 IF (ABS(VA).LT. 0.00008)  GO TO 99
   31 IF ( (VNT(J).GT. 1.27*1.E-7) .OR. (VA.LT. 0.) )  GO TO 6
      IF (VNT(J) .EQ. FLOOR)  GO TO 99
      DX = -VNT(J) + FLOOR
      GO TO 97
    4 IF (VNT(J) .EQ.0.)  GO TO 44
      IF(VA+VNT(NP) .LT. +5.)GO TO 66
      V = EXP(-VA -VNT(NP))
      XMMM = AMIN1(-XMIN, XMAX)
      IF (VNT(J)/XMMM .LT. .01) XMAX=.011*XMMM
      IF ((V+VNT(J))/XMMM .GT. .01)  GO TO 66
      GO TO 45
   44 V = FLOOR
      GO TO 5
   45 V= AMAX1(V,FLOOR)
    5 VTEQ = ABS(1. - VNT(J)/V)
COMMENT MINOR SPECIES TOLERANCE
      IF (VTEQ .LT. .0008)  GO TO 99
   55 DX = V - VNT(J)
      LL(J) = 0
      VNT(J) = V
      GO TO 82
   66 VA= VA+ ALOG(VNT(J)) + VNT(NP)
      IF (ABS(VA) - .0008)  99,99,67
   67 VB = 1.0/VNT(J)
    6 DO  69  I = 1,IS
      IF (X(I))  68,69,68
   68 K = IOJ(I)
      VB = VB + X(I)*X(I)/VNT(K)
```

```
 69 CONTINUE
    VF=0.
    IF (KR(16) .EQ. 0)  GO TO 801
    M=0
    IF (J .LE. IG) M=+1
    VS=SD(J)
    DO 800  I=1,IS
    K=IOJ(I)
    IF (K .LE. IG)  M=M -VNU(J,I)
800 VS=VS-VNU(J,I)*SD(K)
    VF=AMAX1(0., M/FN/1.9871 *VS)
    IF(VF .GT. .5*VB)  VFF=1.5
    IF (VF .GT. VB) VFF=3.
    IF (VF .GT. 1.5*VB) VFF=5.
    VF=VFF*VF
    IF (KR(12) .NE. 0) WRITE (6,802) J,M,VF,VB,PR,VA
802 FORMAT (2I6, 1P 5E12.3)
801 IF (VB.NE. 0.)  GO TO 72
 70 VB = .000C001
    VQ = .999999
 72 DX =-VA/(VB*VF)
    DX= AMAX1(DX, -VQ*VNT(J))
    LL(J) = 9
 97 DX= AMAX1(DX, VQ*XMIN)
    DX= AMIN1(DX, VQ*XMAX)
    IF (ABS(DX) .LT. .0001*VNT(J))  GO TO 81
3465 FORMAT (I5,1P 13E10.3)
 80 CALL SLITE (9)
    IC = 1
 81 VNT(J) = VNT(J) + DX
 82 VC = .99*VNT(J)
    DO 96  I = 1,IS
    IF (VNU(J,I).EQ. 0.)  GO TO 98
975 K = IOJ(I)
    VNT(K) = VNT(K) - VNU(J,I)*DX
    IF (VNT(K) .GE. VC) GO TO 98
    IF(KICK .EQ. 1  .AND.  VNT(K) .GT. VD) GO TO 96
    VD=VNT(K)
    KICK = 1
    JJ = J
    II = K
    KK = I
 96 CONTINUE
    IF (KICK .NE. 1)  GO TO 99
    CALL TABLO(II,JJ,KK)
 99 CONTINUE
100 IF (KR(15).NE.1)  GO TO 107
999 WRITE (6,88)(LL(JJ), JJ = 1,N)
 88 FORMAT (1HO80I1)
107 CONTINUE
    RETURN
    END
```

Appendix I

LISTING OF THE XEP SUBROUTINES

The following listing shows routines which modify the PEP program to evaluate gaseous detonation processes. Only those routines not common to PEP appear. XEP is run the same way as PEP except:

1. Option 9, the input of ingredients by serial numbers is not allowed.
2. Ingredient densities must be inputted as grams/liter instead of lbs/in^3.
3. The first pressure in the weight ratio card is a *guess* for the detonation pressure. It must exceed the second pressure which is the pressure to which the detonation products are expanded.
4. A plot is generated by this program. The plot is only a convergence check and may be deleted.

```
      SUBROUTINE HUGO(PP,HE,V,PONE,TONE,HF,VONE,SONE,HONE)
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(200), W47, NAME, SER
     3COMMON /IPRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), CA,
     4TAU, H(200), SU(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     5IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     6RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     7,LL(200)
      TUPP=6000.0
      TLOW=298.16
      KR(17) = 1
      VNT(NP) = ELOG(1.9871*TONE/VONE)
      CALL EQUIL(TONE,PONE,HONE,SONE,1)
      PONE = FN*VNT(NP)
      Z=HE-HONE-(VONE+V)*(PP-PONE)/2.0
      ZP = Z
      DO 8 J = 1,23
      CF= AMAX1(1.0,CF)
      CF = AMIN1(16.0, CF)
      CV = CP - 1.9871*FN
      DELTAT = +Z/CV/CF
      DELTAT=AMIN1(DELTAT,.5*(TUPP-TONE))
      DELTAT=AMAX1(DELTAT,.5*(TLOW-TONE))
      TONE = TONE+DELTAT
      IF(ABS(DELTAT)-.001)10,88,88
   88 VNT(NP) = ELOG(1.9871*TONE/VONE)
    4 CALL EQUIL(TONE,PONE,HONE,SONE,1)
      PONE = FN*VNT(NP)
      Z=HE-HONE-(VONE+V)*(PP-PONE)/2.0
      CF = ((ZP-Z)/(CV*DELTAT))
      ZP = Z
      CALL SLITET(3,KOUNFX)
       GO TO(70,74),KOUNFX
   74 IF(Z)72,10,71
   71 TLOW=TONE
      GO TO 70
   72 TUPP=TONE
   70 CONTINUE
    8 CONTINUE
   10 HONE = HONE + Z
      SONE = SONE + Z/TONE
      KR(17) = 0
      IF (V .EQ. VONE)  GO TO 903
      HR=((VONE/V)**2*HF-HONE)/((VONE/V)**2-1.0)
  903 RETURN
      END
```

```
      SUBROUTINE PUT IN (LE)
     1COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      COMMON/ICINFO/AAAA(6)
      COMMON ITAG(100), WING(10)
      DIMENSION ATWT(100), SWING(10), VOUT(10)
      DATA IRUN/0 /
      DATA (ATWT(I), I = 1,100)/1.008, 4.003, 6.94, 9.013, 10.82, 12.011
     1,14.008, 16., 19., 20.183, 22.991, 24.32, 26.98, 28.09, 30.975,
     2 32.066, 35.457, 39.944, 39.1, 40.08, 44.96, 47.9, 50.95, 52.01,
     4 54.94, 55.85, 58.94, 58.71, 63.54, 65.38, 69.72, 72.6, 74.92,
     5 78.96, 79.916, 83.8, 85.48, 87.63, 88.91, 91.22, 92.91, 95.95,
     6 99., 101.1, 102.91, 106.4, 107.88, 112.41, 114.82, 118.7, 121.76,
     7 127.61, 126.91, 131.3, 132.91, 137.36, 138.92, 140.13, 140.91,
     8 144.27, 147., 150.35, 152., 157.26, 158.93, 162.51, 164.94, 167.2
     97, 168.94, 173.04, 174.99, 178.50, 180.95, 183.86, 186.22, 190.2,
     1 192.2, 195.09, 197., 200.61, 204.39, 207.21, 208.99, 210., 210.,
     2 222., 223., 226., 227., 232., 231., 238., 237., 242., 243., 247.,
     3 249., 251., 254., 253.  /
    1 FORMAT (19I1, A1, A6, I4, I5, I5)
    2 FORMAT (5A6, 6(F3.3, A2), F7.0, F6.0, I7)
    3 FORMAT (12F6.6, A6, A2)
    4 FORMAT (/1H 34X, 12A6)
    5 FORMAT (12H+INGREDIENTS 79X, 29H     WEIGHT    CAL./G.  DENSITY)
    6 FORMAT (12F10.6)
    7 FORMAT (1H )
    8 FORMAT (1H 5A6,1X, 12F5.3, F9.3, F10.0, F9.4)
    9 FORMAT (43HOGRAM ATOM AMOUNTS FOR PROPELLANT WEIGHT OF F9.3)
   10 FORMAT (1HO 12(4H    (A2,4H)    ))
      LE = 0
      IF (IPUN)  19,11,19
   11 READ (5,1) (KR(I), I = 1,19),ISERI(1), ISERI(2), IN, IT, IRUN
      DO 12  I = 1,12
   12 JAT(I) = 0
      DO 13  I = 1,IN
   13 READ (5,2) (BLOK(I,J), J= 1,5), (FIE(I,J), IE(I,J), J = 1,6),
     1 DH(I), RHO(I)
      CALL STORCH(LE)
      DO 14  I = 1,IN
      WATE(I) = 0.
      DO 14  J = 1,IS
      K = JAT(J)
   14 WATE(I) = WATE(I) + AMAT(I,J)*ATWT(K)
      CALL SEARCH(LE)
      REWIND 12
C     THE NEXT 8 CARDS CONTROL THE SC 4020 OUTPUT ON PSEUDO UNIT 16
   19 CALL CAMRAV(1)
      CALL FRAMEV
      CALL CAMRAV(2)
      CALL FRAMEV
      INC = 1019/(30 + IN + (N+3)/4)
      CALL SCOUTV(1,INC)
      CALL LOCSTV(33,1009,4)
      CALL MAXFRM(5000)
      IF (KR(6) .NE. 1)  GO TO 18
      READ (5,17)
      WRITE (16,17)
   17 FORMAT (60H
     1                                                            )
   18 READ (5,3) W1(5), W1(6), (WING(I), I = 1,10),ISERI(3), ISERI(4)
      WRITE (6,16) (ISERI(I), I = 2,4)
   16 FORMAT (1H1 3A6)
```

```
      IF (KR(2) .NE. 1)  GO TO 20
      IS = IS -1
   2L IRUN = IRUN - 1
      KR(19) = 1
      IF (WING(1) .EQ. 0.)  GO TO 120
      KR(19) = 0
      DO 21  J = 1,IS
      ALP(J) = 0.
      DO 21  I = 1,IN
   21 ALP(J) = ALP(J) + AMAT(I,J)*WING(I)/WATE(I)
      W27 = 0.
      W1(4) = 0.
      W43 = 0.
      VA = 1.
      DO 22  I = 1,IN
      SWING(I) = WING(I)
      W1(4) = W1(4) + DH(I)*WING(I)
      W27 = W27 + WING(I)
      IF (RHO(I))  25,25,24
   24 W43 = W43 + WING(I)/RHO(I)
      GO TO 22
   25 VA = 0.
   22 CONTINUE
      W43 = VA/W43  *W27
  120 IF (KR(4) .NE. 1)  GO TO 23
      IF (KR(17) .EQ. 1)  GO TO 23
      W1(5) = W1(5)/14.7UU69
      IF (KR(7) .EQ. 1)  GO TO 23
      W1(6) = W1(6)/14.7UU69
   23 WRITE (16,4) (ASPEC(I), I = 1,IS)
      WRITE ( 6,4) (ASPEC(I), I = 1,IS)
      WRITE (16,5)
      WRITE ( 6,7)
      WRITE (16,7)
      DO 27  I = 1,IN
      IF (KR(5) .NE. 0)  GO TO 27
      WRITE ( 6,8)(BLOK(I,J), J = 1,5), (AMAT(I,J), J = 1,12),SWING(I),
     1DH(I), RHO(I)
   27 WRITE (16,8)(BLOK(I,J), J = 1,5), (AMAT(I,J), J = 1,12),SWING(I),
     1DH(I), RHO(I)
   36 FORMAT (20HCXEP VOLUME RATIOS = 10F10.5)
      SU = 0.
      DO 34  I = 1,IN
   34 SU = SU + WING(I)/RHO(I)
      DO 35  I = 1,IN
   35 VOUT(I) = WING(I)/RHO(I)/SU
      WRITE (16,36) (VOUT(I), I = 1,IN)
      WRITE ( 6,9) W27
      WRITE (16,9) W43
      WRITE ( 6,10) (ASPEC(I), I = 1,IS)
      WRITE (16,10) (ASPEC(I), I = 1,IS)
      WRITE ( 6,6) (ALP(I), I = 1,IS)
      WRITE (16,6) (ALP(I), I = 1,IS)
      IF (KR(2) .NE. 1)  GO TO 28
      IS = IS + 1
   28 IF (LE .NE. 1)  GO TO 29
      IF (IRUN .EQ. 0)  GO TO 29
      DO 30  I = 1,IRUN
   30 READ (5,1)
      WRITE ( 6,33)
      IRUN = 0
   33 FORMAT (52HOMAYBE THIS TIMID MONITOR WILL TRY THE NEXT SYSTEM.  )
   29 RETURN
      END
```

```
      SUBROUTINE PVPLOT
     0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     4,LL(200)
      COMMON/EXPLO/ VL(20), PL(20), VEL(20), HT(20), TET(20), NE
      CALL GRIDIV (1, .2, 1., 0., 6000., .01, 100., 10,10,10,10,3,4)
      DO 19  I = 1,NE
      IX1 = IX2
      IP1 = IP2
      IS1 = IS2
      IV1 = IV2
      IC1 = IC2
      IX2 = NYV(VL(I))
      PL(I) = PL(I)*100.
      HT(I) = HT(I)/10.
      IP2 = NYV(AMIN1(PL(I), 6000.))
      IS2 = NYV(AMIN1(HT(I), 6000.))
      IV2 = NYV(AMIN1(VEL(I),6000.))
      IC2 = NYV(AMIN1(TET(I), 6000.))
      IF (I.EQ.1)  GO TO 19
      CALL LINEV(IX1,IP1,IX2,IP2)
      CALL LINEV(IX1,IS1,IX2,IS2)
      CALL LINEV(IX1,IC1,IX2,IC2)
      IF (I .EQ. NE)  GO TO 19
      CALL LINEV(IX1,IV1,IX2,IV2)
   19 CONTINUE
      CALL APLOTV(30, VL,   PL, 9,9,1, 1HP, NLAST)
      CALL APLOTV(30, VL,  TET, 9,9,1, 1HT, NLAST)
      CALL APLOTV(30, VL,  VEL, 9,9,1, 1HV, NLAST)
      CALL APLOTV(30, VL,   HT, 9,9,1, 1HH, NLAST)
      CALL PRINTV(33, 33HVOLUME RATIO ALONG HUGONIOT CURVE, 416.6 )
      CALL APRNTV (0,-16, 61, 61H*PRESSURE X100    *TEMPERATURE    *VELO
     1CITY    *ENTHALPY /10  ,4, 592)
      RETURN
      END



CMAIN PROGRAM
      0COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
      1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
      2ISERI(10), WATE(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
      0COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
      1TAU, H(200), SD(200), Y(200), JC, IR(200,2), DMU(200), VLNK(200),
      2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
      3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
      4,LL(200)
       COMMON/EXPLO/ VL(20), PL(20), VEL(20), HT(20), TET(20), NE
       COMMON/MUON/TSTEST,TE
    77 0FORMAT(19HOINITIAL DENSITY = ,F12.6,6X,19HINITIAL PRESSURE = F12.6
      1/23HODETONATION PRESSURE = ,F12.5,6X,22HDETONATION VELOCITY = ,F12
      2.5)
    66 0FORMAT(19HOHEAT OF REACTION =,F11.2,13X,19HPARTICLE VELOCITY =,F12
      1.2)
    33 0FORMAT(36HO1MPULSE FROM ISENTROPIC EXPANSION= ,F14.5)
  8888 CONTINUE
     8 CALL PUT IN (LE)
       PIN = W1(6)
       HIN = W1(4)
       VIN = 1.9871*W27/643/.8205
```

```
      TE=3000.0
      CALL GUESS(TE,PIN)
      CALL CODET (VMIN)
      CALL HUGO(PIN,HIN,VIN,PZERO,TE,HRZERO,VMIN,SZERO,HZERO)
      TCH=TE
      HE = HIN
  803 VWAVE=SQRT(8372.0*(HRZERO-HE)/W27)
  905 LS = 1
      CALL OUT (PZERO, TE, HZERO, SZERO, LS)
      PR = PIN
  906 WRITE(16,77)W43,PR,PZERO,VWAVE
      WRITE( 6,77)W43,PR,PZERO,VWAVE
  907 SOUNDV=SQRT(8372.0*(HRZERO-HZERO)/W27)
      PARTV=VWAVE-SOUNDV
      SYSENT=SZERO
      CALL S PAL (TE, PR, HE, SYSENT, TCH, 1)
      OHE=HE
      CALL EQUIL(298.16,PR,HE,ENTR,0)
      OHREAC = (HZERO - HE)/1000.
      WRITE(16,66)OHREAC,PARTV
      WRITE( 6,66)OHREAC,PARTV
      FSI = 9.3294*SQRT((HZERO - OHE)/W27)
      WRITE(16,33)FSI
      WRITE( 6,33)FSI
 1010 CONTINUE
      CALL PVPLOT
      GO TO 8888
      END
```

```
      SUBROUTINE CODET (VMIN)
     COMMON A(12,12), KR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WAT(10), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     COMMON /IBRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), GA,
     1TAU, H(200), SU(200), Y(200), JC, IP(200,2), DMU(200), VLNK(200),
     2IOU(12), RA(20,  ), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CI    ,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     4,LL(200)
      COMMON/EXPLO/ VL(20), PL(20), VEL(20), HT(20), TET(20), NE
      COMMON/MOON/TSTEST,TONE
      PIN = W1(6)
      HIN = W1(4)
      VIN = 1.9871*W27/W43/.08205
      VONE = VIN
      CALL HUGO (PIN, HIN, VIN, PONE, TONE, HRONE, VONE, SONE, HONE)
      VL(2) = 1.
      PL(2) = PONE
      VEL(2) = +1000.0000000.
      HT(2) = HONE-HIN
      TET(2) = TONE
      VONE = .55*VIN
      CALL HUGO (PIN, HIN, VIN, PONE, TONE, HRONE, VONE, SONE, HONE)
      VL(1) = .55
      PL(1) = PONE
      VEL(1) = SQRT(8372.*(HRONE-HIN)/W27)
      HT(1) = HONE-HIN
      TET(1) = TONE
      NE = 2
      DL = .25
      IM = 1
      DO 19  K = 1,9
      NEM = NE-1
```

```
      DO 12    I = IM,NE
      IL = NE + 2 + IM - I
      VL(IL) = VL(IL-2)
      PL(IL) = PL(IL-2)
      TET(IL) = TET(IL-2)
      VEL(IL) = VEL(IL-2)
   12 HT(IL) = HT(IL-2)
      VL(IM+1) = VL(IM)
      PL(IM+1) = PL(IM)
      TET(IM+1) = TET(IM)
      HT(IM+1) = HT(IM)
      VEL(IM+1) = VEL(IM)
      VL(IM+2) = VL(IM+1) + DL
      VL(IM) = VL(IM+1) - DL
      IL = IM +2
      DO 15  J = IM,IL,-1
      VONE = VL(J)*VIN
      CALL HUGO (PIN, HIN, VIN, PONE, TONE, HRONE, VONE, SONE, HONE)
      PL(J) = PONE
      VEL(J) = SQRT(8372.*(HRONE-HIN)/W27)
      TET(J) = TONE
   15 HT(J) = HONE - HIN
      A1 = VEL(IM+1)
      A2 = (VEL(IM+2)-VEL(IM))/2./DL
      A3 = (VEL(IM) + VEL(IM+2) - 2.*VEL(IM+1))/2./DL/DL
      VMINP = VMIN
      VMIN = VL(IM+1) - A2/3./A3
      DELP = DEL
      DEL = ABS(VMIN-VMINP)
      DO 17  I = 1,2
      IF (VEL(IM) .LT. VEL(IM+1))  GO TO 18
   17 IM = IM +1
   16 NE = NE + 2
   19 DL = DL/2.
      VMIN = VMIN*VIN
      RETURN
      END
```

Appendix J

SUBROUTINE VERSION OF PEP

By exchanging the main program and input routine with the subroutines below, one obtains a version of the program that may be made a satellite of another main program. This has been done for the final reduction program for airbreathing propulsion tests.[15]

```
      SUBROUTINE PEPS
     0COMMON A(12,12), KK(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(4,5), W1(6), W43, IG, NP, VNT(201), W47, NAME, SER
     0COMMON /IRRIUM/ TL(200,2), TU(200,2), W3(200), VNU(200,12), QA,
     1TAU, H(200), SO(200), Y(200), JC, IP(200,2), DMU(200), VLNK(200),
     2IOJ(12), RA(200,2), RB(200,2), RC(200,2), RD(200,2), RE(200,2),
     3RF(200,2), CH(200,2), JM, W48, CP, FN, C(12,200), SPECIE(200)
     4,LL(200)
      COMMON/MOON/TSTEST,TE,IRUN
      COMMON/RESULT/SP1(2),AST(2),GAM(2),CF(2),EV(2),RISP(2),OEX(2),
     XTHRT(2),TEX(2),TCOMB,ENTH(2),ENTRO(2),GASM(2),RTV(2)
      TCH = 3467.
      TE= AMAX1(TCH, 500.0)
      TSTEST = 0.
      TE = AMIN1(TE,5000.)
      PR=W1(5)
   15 IF (KP(7) .EQ. 0)  GO TO 14
      TE = W1(6)
      VNT(NP) = ELOG(.0F205*W1(6)/W1(5))
      CALL EQUIL (TE, PR, HE, SE, 1)
      PR = FN*VNT(NP)
      SYSENT = SE
      GO TO 8
   14 CALL H BAL (TE, PR, SYSENT, 1)
   12 TCH = TE
      TCOMB=TCH
      ENTH(1)=W1(4)
      ENTRO(1)=SYSENT
      GASM(1)=FN
      RTV(1)=VNT(NP)
      GAM(1)=CP/(CP-FN*1.9671)
      GASM(2)=0.
      IGP=IG+1
      DO 1  I=IGP,N
    1 GASM(2)=GASM(2)+VNT(I)
    8 RETURN
      END
```


[15] Naval Weapons Center. *The Final Reduction Program for Airbreathing Propulsion Tests at T-Range, Theory and Usage*, by L. R. Cruise. China Lake, Calif., NWC, January 1978. (NWC TM 3364, publication UNCLASSIFIED.)

```
      SUBROUTINE  PUTINS(ISER,WTS)
      DIMENSION ISER(10), WTS(10)
     0COMMON A(12,12), PR(20), AMAT(10,12), JAT(12), ASPEC(12), IN, IS,
     1FIE(10,6), IE(10,6), ALP(12), W27, N, BLOK(10,5), DH(10), RHO(10),
     2ISERI(10), WATE(10), WI(6), W43, IG, NP, VNT(201), W47, NAME, SER
      COMMON ITAG(100), WING(10)
      COMMON/ILINFO/AAAA(6)
      DIMENSION ATWT(100), SWING(10)
      COMMON/MOON/TSTEST,TE,IRUN
      DATA (ATWT(I), I = 1,100)/1.008, 4.003, 6.94, 9.013, 10.82, 12.011
     1,14.008, 16., 19., 20.183, 22.991, 24.32, 26.98, 28.09, 30.975,
     2 32.066, 35.457, 39.944, 39.1, 40.08, 44.96, 47.9, 50.95, 52.01,
     4 54.94, 55.85, 58.94, 58.71, 63.54, 65.38, 69.72, 72.6, 74.92,
     5 78.96, 79.916, 83.80, 85.48, 87.63, 88.91, 91.22, 92.91, 95.95,
     6 99., 101.1, 102.91, 106.4, 107.88, 112.41, 114.82, 118.7, 121.76,
     7 127.61, 126.91, 131.3, 132.91, 137.36, 138.92, 140.13, 140.91,
     8 144.27, 147., 150.35, 152., 157.26, 158.93, 162.51, 164.94, 167.2
     97, 168.94, 173.04, 174.99, 178.50, 180.95, 183.86, 186.22, 190.2,
     1 192.2, 195.09, 197., 200.61, 204.39, 207.21, 208.99, 210., 210.,
     2 222., 223., 226., 227., 232., 231., 238., 237., 237.,12.01,9.031,
     310.82,24.32,26.98, 253.  /
      LE = 0
      IF (IRUN .NE. 0)  GO TO 19
   11 DO 12  I = 1,12
   12 JAT(I) = 0
      KP=1
      REWIND 11
      READ(11,1110)VA
      DO 13  I = 1,IG
      K=ISER(I)
      IF (KP .LT. K)  GO TO 1117
      REWIND 11
      READ(11,1110)VA
      KP=1
 1117 DO 1113 J=KP,K
 1113 READ (11,1110)(VNT(L),L=1,12)
 1110 FORMAT (11A6,A5)
      KP=K+1
 1115 CONTINUE
   13 DECODE(2,VNT)(BLOK(I,J),J=1,5),(FIE(I,J),IE(I,J),J=1,6),
     1 DH(I), RHO(I)
```

```
    2 FORMAT (5A6, 6(F3.3, A2), F5.0, F6.0, I7)
      CALL STOICH(LE)
      DO 14  I = 1,IN
      WATE(I) = 0.
      DO 14  J = 1,IS
      K = JAT(J)
   14 WATE(I) = WATE(I) + AMAT(I,J)*ATWT(K)
      CALL SEARCH(LE)
   16 IF (KR(2) .NE. 1)  GO TO 19
      IS = IS -1
   19 DO 1199 I=1,IN
 1199 WING(I)=WTS(I)
   20 KR(19) = 0
      DO 21  J = 1,IS
      ALP(J) = 0.
      DO 21  I = 1,IN
   21 ALP(J) = ALP(J) + AMAT(I,J)*WING(I)/WATE(I)
      W27 = 0.
      W1(4) = 0.
      W43 = 0.
      VA = 1.
      DO 22  I = 1,IN
      SWING(I) = WING(I)
      W1(4) = W1(4) + DH(I)*WING(I)
      W27 = W27 + WING(I)
      IF (RHO(I))  25,25,24
   24 W43 = W43 + WING(I)/RHO(I)
      GO TO 22
   25 VA = 0.
   22 CONTINUE
      W43 = VA/W43  *W27
  120 IF (KR(4) .NE. 1)  GO TO 23
      IF (KR(17) .EQ. 1)  GO TO 23
      W1(5) = W1(5)/14.70069
      IF (KR(7) .EQ. 1)  GO TO 23
      W1(6) = W1(6)/14.70069
   23 DO 27  I = 1,IN
   27 IF (KR(2) .NE. 1)  GO TO 28
      IS = IS + 1
   28 CALL GUESS(2500.,50.)
   29 RETURN
      END
```

NOMENCLATURE

Note: Symbols are listed in the order of their appearance in text.

S	Number of chemical elements
N	Number of molecular species ($N \geqslant S$)
C	Molecular composition matrix
c_{ik}	Elements of composition matrix
$i(j)$ $1 \leqslant j \leqslant S$	A given choice of basis species
$b_{jk} = c_{i(j),k}$	Composition matrix of basis species
$n_{i(j)}$	Molar amounts
B	Optimized basis matrix
b_{jk}	Element of basis matrix
ν	Matrix of reaction coefficients
K_i	Equilibrium constant for ith reaction
g_i	Gibbs free energy for ith species
R	Gas constant (1.9871 cal/K-mole = 0.08205 ℓ-atm/K-mole)
T	Temperature
$\Delta\xi$	Small difference in reaction coordinate
n_i	Molar amounts
n_i'	New composition after adjustment of n_i
$\gamma_{i(j)}$	Phase parameter $\left\{ \begin{matrix} 1 \text{ for gas} \\ 0 \text{ for condensed} \end{matrix} \right\}$ for ith species
A	$P/\sum_{i=1}^{N} = RT/V$
P	Pressure
Q_i	Guess for equilibrium constant
$f(T)$	$H(T) - H_O$ or $S(T) - S_O$ in enthalpy or entropy balance procedure
$H(T)$	Enthalpy at temperature T
H_O	Reference enthalpy
$S(T)$	Entropy at temperature T
S_O	Reference entropy
C_p	Specific heat at constant pressure
K	Degrees Kelvin
H_1, V_1, T_1, S_1, P_1	Chamber state variables
H_2, V_2, T_2, S_2, P_2	Exit plane state variables

V_1, V_2	Volume
I_{sp}	Specific impulse
g_{MKS}	Acceleration of gravity in SI units
J	Mechanical equivalent of heat
m	Mass
γ	C_p/C_v = ratio of specific heats
L	Conversion factor
γ_c	A parameter that equals γ only for a perfect gas
γ_v	Isentropic exponent ($PV^{\gamma v}$ = constant). A parameter that equals γ only for a perfect gas
$\dot{m}$	Mass flow
k	10^3 liters/m^3
ρ	Density
v	Velocity
A	Duct cross-sectional area
P^*, A^*	Nozzle throat values
C_f	Throat coefficient
C^*	Characteristic velocity
g_{FPS}	Acceleration of gravity in common units
ΔU	Ideal boost velocity
g	Acceleration due to gravity
ρ^*	Switch density

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